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A.K.Rebrov, V.Ya.Rudyak, A.A.Belkin

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1, Ul. Lavrent'eva
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The results of theoretical and experimental investigations on the following topics are given in the papers: kinetic theory, non-equilibrium statistical mechanics, irreversibility and dynamic chaos, transport processes and relaxation phenomena in gases and liquids, gas-surface interaction, methods of solving the kinetic equations, gas and liquid simulation methods, rarefied gas dynamics, physics and dynamics of clusters and aerosols.

The issue is meant for specialists in the field of kinetic theory, continuum mechanics, non-equilibrium processes physics, as well as for students and post-graduate students of the corresponding specialties.

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Kinetic Theory and Rarefied Gas Dynamics

Book of Abstracts of All-Russia Seminar

December 2 to 7, 2002

The seminar is devoted to the 130th anniversary of the publication of the Boltzmann equation

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PREFACE

The present Seminar is devoted to the 130th anniversary of publishing the Boltzmann equation and H-theorem. An extensive interdisciplinary scientific trend, including the kinetic theory, statistical mechanics, theory of transport processes in gases, liquids and plasma, theory of relaxation phenomena, has been formed on the basis of Boltzmann's ideas today. The kinetic theory methods have been developed especially actively during the last four decades of the previous century in connection with various space applications. The International Symposium on Rarefied Gas Dynamics, held regularly for about 50 years, witnesses the active development of the kinetic theory and the dynamics of rarefied gas. More than 10 conferences in this field were also held in the former Soviet Union. The last of them took place in 1991. Holding of a similar conference in Russia now will make a new impact on further development of the above-mentioned scientific trends. The present Seminar is focused on the following topics:

1. The Kinetic Theory and Non-Equilibrium Statistical Mechanics.
2. Irreversibility and Dynamic Chaos.
3. Transport Processes and Relaxation Phenomena in Gases and Liquids.
4. Gas-Surface Interaction.
5. Mathematical Methods in Kinetic Theory.
6. Modeling Methods in Rarified Gas Dynamics.
7. Rarified Gas Dynamics.

The program of the Seminar provides for four round-table discussions on the topics:

- Irreversibility and Dynamic Chaos.
- Numeric Methods of Solving the Boltzmann Equation and Monte Carlo Methods.

- The Problems of Kinetic Description of Rarefied Plasma.
- The Place of Kinetic Theories in the Development of High Technologies, in Particular, Nanotechnologies.

The objectives of the Seminar: (i) renewal of the representative conference in the given research field in Russia; (ii) involvement of young investigators, post-graduate and undergraduate students to the given scientific topic; (iii) exchange by the latest scientific achievements; (iv) critical comprehension of achievements and problems encountered in the given scientific field today.

We find it a pleasant duty to express our sincere gratitude to the organizations and funds, which gave financial support to the seminar. They are EOARD, RFBR and FSP "Integration".

A.K. Rebrov
V.Ya. Rudyak

Ludwig Boltzmann

LUDVIG BOLTZMANN AND KINETIC GAS THEORY

Rudyak V.Ya.
Novosibirsk State University of Architecture and Civil Engineering,
rudyak@ngasu.nsk.su

1. Introduction

Looking back at the history of science, one can see only the works, which have borne the fruit of today's knowledge. According to their ideas they can be divided into two classes. To the first one we can refer the works, radically changing our notions of the universe. The concepts of Newton's classic mechanics belong to this class, as well as the concepts of Maxwell's electrodynamics, Einstein's relativistic mechanics, Schrodinger's-Bohr's-Heisenberg's quantum mechanics. The other class is represented by the works, in which new methods of describing facts, proved experimentally, are created. Both classes have equal importance, because knowledge acquires the form of scientific truth only when it is expressed with the language of mathematical methods. Often it is impossible to divide works into these two classes. This is just the case, when we analyze scientific heritage of L. Boltzmann. His scientific work is rather big and versatile. There are both experimental and theoretical works here, which have become landmarks of the XIXth century classic physics. The Hall effect theory, created by Boltzmann, can be referred to such works. Among them there is also dielectric constant measurement of some gases. Nevertheless, perhaps, the most important thing in his investigations was an attempt of creating a unified physical theory, combining then existing mechanics, thermodynamics, hydrodynamics, etc. Today we may say, that Boltzmann tried to derive physical laws "from the first principles".

More than a century has passed since that time, but still today, when real brilliant results proved his approach to be fruitful, this approach is treated with tense, preconceived opinion and distrust. It's small wonder that in the 70^{s} of the century before last, his theory was not appreciated, especially if to take into account that Boltzmann unique physics theory was based on mechanics of atom and molecule substance, while scientific community had not agreed to the existence of atoms and molecules! With all this he inevitably came to the concept of statistic description of a system with a lot of interacting particles, thus having proved to be the forefather and creator of the statistic physics, statistic mechanics, statistic thermodynamics, thermodynamics of irreversible processes. May be it's a paradox, that the logic of building the theory made Boltzmann to come over from a determinative mechanistic description of the system to a probability description. And only today, at the beginning of the XXI century, having absorbed the knowledge of the dynamic systems theory we come to understanding of the clarity of his vision and farsightedness of this step.

How and thanks to what are such spurts realized? This question is not futile; this is the question of methodology. Probably we cannot answer it yet, but we can try to find some substitute for the answer, having analyzed some landmarks of the investigator's life. It's good timing for this on the conference, devoted to 130 anniversary of publishing the H-theorem and the Boltzmann equation.

2. Biographical Data

Ludvig Boltzmann was born in February 20, 1844 to a rather well to do family. However, his childhood was darkened with some tragedies, which practically ruined the family; early death of his father, his younger brother and his sister. L. Boltzmann spent his school years in Linz. He was doing well and he was ambitious. The boy's ambitions were limited with the traditional family fields: business, practice as a barrister, science. Ludvig chose the last and began studying physics at Vienna University at the age of 19. With 21 y. o. he published his first work, and one year later the article "About the Mechanical Significance of The Second Law of The Heat Theory" appeared. The sphere of Boltzmann's scientific interests had been determined and remained invariable all his life.

What made Boltzmann seek the perfection of physics theories in atomic-molecular nature of substance? Surely, it was infinite confidence in atomism, which had become a working concept in chemistry by the time, though had not yet had any evident proofs in physics. Absence of these proofs in Boltzmann's mind was compensated by charm and perfection of mechanics, which acquired new exquisite style of analytical theory. There was one more circumstance, I think. Young L. Boltzmann was romantic, immersed in music and poetry.

Beauty was quite material for him, he could feel music of poetry and perfection of lines. And what can be more perfect than gas heat theory, based on mechanics of molecules movement?

L. Boltzmann defended his Doctor's theses at Vienna University in 1866, and worked as an assistant with J. Stefan for 2 years. 3 years later he moved to Graz, having acquired mathematical physics professorship in this city for the first time in his life (at the age 25!). It was the peak of Boltzmann's creative ability. At that time his famous equation appeared and H-theorem was stated. The amount of his academic work leaved Austrian professor enough time for serious scientific investigation and intercourse with colleagues. Academic mobility, which has been discussed in Russia at the Ministry of Education for two years, was well known in Austria in the XIX century. His two semester leaves in 1871 and 1872 L. Boltzmann spent in Geidelberg and Berlin. In the former he worked with R.B. Bunsen and L. Kenigsberger, and in the later he worked with G.R. Kirchhoff and G. Helmholtz.

In 1873 he came back to Vienna University and spent there three years, but then there was again Graz and his marriage, he married Henrietta von Eigentler, whom he had got acquainted with during his previous visit. She was ten years younger than Ludvig and then was a student of mathematic faculty of the University. His academic career was quite successful and accompanied by comings out. Theatre was of great importance in his life, from time to time, keeping tradition of Vienna period; they set up musical evenings, and Boltzmann himself played the piano with pleasure. Sunday picnics were not rare in the picturesque suburbs of Graz. Boltzmann's reputation was generally recognized, in 1878 he became the dean of the faculty, in 1885 – member of Vienna Science Academy, and in 1887 – president of the University.

Graz period was exceptionally fruitful. Intensive development and comprehension of basic ideas of gas kinetic theory and their use in overlapping field of physics was going on. An outstanding result, acquired in this way, was the justification of the law of the black-body radiation, Stefan-Boltzmann law, as it is called today.($I \sim T^4$, here T is temperature).

In 1890 L. Boltzmann was appointed to the Chair of Theoretical Physics in Munich University. It was the end of his quiet life. Four years later he inherited the Chair of Theoretical Physics in Vienna University after his teacher Y. Stefan and came back to Vienna. Then there was Leipzig, not for long, and again Vienna, till the end of his life that time.

The last period of his life was also very meaningful. He lectured a lot. In Vienna University he was lecturing a four years course of physics (!), which included mechanics, theory of elasticity, hydrodynamics, electrodynamics and kinetic gas theory. Boltzmann's scientific interests were concentrated on philosophy more and more. Philosophy became his profession, especially after his appointment to the Chair of Naturphilosophy after E. Mach in 1903. He traveled a lot – to Turkey, North Africa, Portugal. But his far-off travels were beyond the ocean. L. Boltzmann visited America three times. In 1899 he delivered four lectures at the University of Worchester, and during his last visit (in 1905) he delivered a course of 30 lectures at summer school of Californian University in Berkeley. He described this travel in his "Reise eines deutschen Professors ins Eldorado".

According to his students opinion L. Boltzmann was a brilliant lecturer and his attitude to teaching was extremely responsible and quivering. Here is what he wrote at the beginning of his book "Principles of Mechanics": "Say only what is true, write so that it was clear, and plant the seeds of knowledge only after they have ripened in you" [1].

And yet only scientific inheritance is left to people. We'll speak about it further.

3. Idea of Statistical Description

Our interests and raptures are determined by Lord, whom we call chance, and by our teacher. J. Stefan, who happened to be L. Boltzman's teacher, made him acquainted with Maxwell's works on kinetic theory[1]. Maxwell's ideas were sown into a fertile soil. As a matter of

[1] L. Boltzmann himself wrote about it as follows: "When being a student I made friends with Stefan, he gave me Maxwell's works, accompanied with English grammar"[2].

fact L. Boltzmann was the first person, who introduced the concept of statistical ensemble, he did it long before J. Gibbs, and after that, determination of macroscopically observed values quite natural, these values were determined as ensemble average from corresponding dynamical variables. L. Boltzmann also considered quite natural the idea of equal microstate probability of ensemble; that is to say, the microcanonical ensemble was meant, in fact. Today microcanonical ensemble is the corner stone of the whole of the statistical physics ("statistical static", as Boltzmann put it [3]).

The appearance of probability description of deterministic Hamilton system by means of distribution function had become the fact, that left then existing scientific notions far behind. Also the situation is typical today, when professionals of physics and mechanics do not understand and do not accept such description. The best is when this description in spoken to be a kind of mathematical apparatus, which has to be used, because of our restricted possibilities of the description of real molecular systems. However, it is not only this fact. At least two circumstances should be mentioned here.

First of all, the traditional thermodynamic and hydrodynamic descriptions of many-particle systems, which prevailed in physics and mechanics of the XIXth century, are feasible only in some stages of their evolution. In some situations it is necessary to make more subtle description, which may be achieved weather at the level of one-particle distribution function or even multi-particle distribution function.

The second circumstance became clear quite recently, after the development of the dynamical system theory. It was found, that local instability of the systems' trajectories of comparatively small perturbations of the initial conditions is characteristic of the dynamics of real molecular systems. At the same time an exact δ-like specification of initial conditions for a multi-particle system is impossible, not only technically, but is also forbidden by the Heisenberg uncertainty principle. Dynamical description is possible only on a rather coarse-grained phase space. Thus, the Newton's description is unpromising. What we really do is to investigate the evolution of the microscopic state distribution function of a system. So it is very likely, that the dynamic system description with the help of the distribution function is

not only the unique technically possible description but also the only realistic one.

Having introduced the distribution function Boltzmann attained one more goal. Thermodynamics of the XIXth century dealt with equilibrium values, and nowadays hot discussions about phenomenological definitions of temperature or entropy of non-equilibrium processes are going on. The introducing of the system description at the level of the distribution function abolished the problem. The theory gives exact definitions of these parameters, being transformed in equilibrium into corresponding thermal analogs. Today's successes of thermodynamics are caused to a great extent with the development of non-equilibrium statistical thermodynamics.

Having recorded the existence of the irreversible non-equilibrium processes by the second low, thermodynamics did not have a mathematical apparatus for their description. These processes were studied in hydrodynamics on the basis of phenomenological transport equations, Euler equations or Navier-Stokes equations. There was a gap between those two theories both in methods and in methodology. The necessity of the development of a universal description method for irreversible processes became urgent. And the first step in this direction was made by the deriving the kinetic equation of rarefied gas – Boltzmann's kinetic equation..

4. Boltzmann Kinetic Equation

The kinetic equation for the distribution function of gas molecules $f(\mathbf{r},\mathbf{v},t)$

$$\frac{\partial f_1}{\partial t}+\mathbf{v}_1\cdot\frac{\partial f_1}{\partial \mathbf{r}_1}=\int d\mathbf{v}_2 d\Omega v_{21}\left[f_1(\mathbf{v}_1')f_1(\mathbf{v}_2')-f_1(\mathbf{v}_1)f_1(\mathbf{v}_2)\right] \qquad (1)$$

appeared in 1872 in Boltzmann's famous work [4], devoted to proving the H-theorem. Here $d\Omega$ - is differential scattering cross-section of molecules. The rest notations are standard ones.

However, significance of the kinetic equation (1) exceeds that of an auxiliary instrument for proving the H-theorem. For this reason the equation's adequacy and the range of its applicability has been being investigated in details for more than a century. Many considered Boltzmann's heuristic derivation unsatisfactory, and numerous at-

tempts were made to derive this equation immediately from Liouville equation. The review of the results obtained here can be found in [5]. Common summary, concerning the suppositions, implied by the Boltzmann's equation derivation, can be listed as follows:

1. Molecules are supposed to be identical and having no structure.
2. Only binary collisions of molecules are taken into account, and consequently, gas is supposed to be rather rarefied.
3. The molecule interaction potential is supposed to be short-range and repulsive.
4. The colliding molecules are supposed to be statistically independent before collision.
5. One-particle distribution functions do not change at distances of the order of the effective interaction radius of molecules and at corresponding times.

G. Uhlenbeck formulated a number of questions concerning possible generalizations of this equation in his conference opening lecture, devoted to the hundred year anniversary of the Boltzmann equation publication, which took place in 1972 in Vienna [6]. Here are some of the questions: (i) Can the Boltzmann's equation be applied to the case of polyatomic gas? (ii) Can the equation for dense gas be derived? (iii) Does the Boltzmann equation describe the fluctuations, taking place in gas? G. Uhlenbeck answered all the 3 questions negatively, though with some provisos. That was the reason for him to characterize the equation with the well-known Boltzmann's phrase, which was pronounced by the later with reference to Maxwell's equation: «Ist es ein Gott, der dieses Zeichen schuf?»[2]. Has our notion changed during the last 30 years?

The kinetic theory of polyatomic gases has been developing intensively during these years, however quantum nature of internal degrees of freedom and consequent conventionality of the corresponding classical models keeps Uhlenbeck's answer unchanged, though from the practical point of view a good deal of concrete results have been achieved.

A great number of publications, beginning with the well-known D. Enskog works, were devoted to the derivation of the dense gas ki-

[2] Free translation of the phrase may sound as: "Is not it Lord's work?"

netic equations. The first regular method of derivation of the kinetic equations as a density series was proposed by N. Bogoliubov [7]. Then another series of methods were proposed with different variations of the initial premises, the review of the methods can be found in [5]. A kinetic equation is derived from a so-called chain of equations BBGKI for s-particle distribution functions $F_s(x_1,...,x_s,t)$. It is virial series solution that is being sought practically by all the methods, and these or those conditions of the correlation attenuation are used here. The latter are presented in Bogoliubov's method as follows

$$\lim_{t\to\infty} S_{-t}^{(s)}\left[F_s(x_1,...,x_s,0)-\prod_i^s F_1(x_i,0)\right]=0 \qquad (2)$$

and postulate statistical independence in the remote past ($S_{-t}^{(s)}$ — system evolution operator of s particles). The condition (2) is generalization of the well-known hypothesis of molecular chaos of L. Boltzmann – Stosszahlansatz.

Practically all methods have met certain difficulties: there are terms growing at time in the higher orders of solution of the kinetic equations. Physically it is connected with the fact that the conditions of attenuation of correlation (2) cannot be applied in dense gas. Here special sequences of molecule collisions appear, in which correlations are kept on times about several times of free pas of molecules. Due to this fact it was proposed in work [8] to use the condition of partial attenuation of correlations

$$\lim_{t-t_0>>\tau_0}\left[S_{-(t-t_0)}^{(s)}F_s(x_1,...,x_s,t_0)-\chi_s(x_1,...,x_s)S_{-(t-t_0)}^{(s)}\prod_i^s F_1(x_i,t_0)\right]=0\,. \qquad (3)$$

Roughly speaking, the condition (3) corresponds to conservation of the persistence of the so-called statistical correlations, which take place in a dense system even in the equilibrium state and which are described by configuration correlation function χ_s. However, this condition is not markovian one, and conservation of some part of dynamic correlations is taken into account in it.

Use of condition (3) allows developing the closed kinetic theory of moderately dense gas without divergence [5, 8]. At the same time,

attempts to develop the kinetic theory of very dense gases and liquids are doomed beforehand, though there were some attempts. Evolution of liquid cannot be described at the level of one-particle distribution function, in principal. Even equilibrium properties of liquid are known to require at least the knowledge of pair distribution function. So, we have to agree with the negative answer, in the respect of the second Uhlenbeck's question.

As to the third question, the situation here demands explanations. The condition of molecular chaos or more general conditions of correlation attenuation (2), (3) exclude from the sphere of consideration of Boltzmann equation longwave kinetic fluctuations. Such fluctuations can be studied within the kinetic theory, but then, some additional fluctuation sources and collision integrals, connected with them will appear in the kinetic equations. For the first time such kinetic equations have been formulated by V.N. Zhigulev [9, 10] and then were studied actively by Yu.L. Klimontowich [11, 12].

At the same time Boltzmann kinetic equation is quite applicable to the description of both kinetic and hydrodynamic processes. During the derivation of hydrodynamic equations, macroscopic variables φ_i are usually determined as first five moments of the distribution function. These variables contain much more information, than the corresponding values in phenomenological theories. If we make the same suppositions, as in usual phenomenological hydroaeromechanics while defining macroscopic variables, we derive transport equations with fluctuation terms [13]. The scale of these source terms turns out to be less or about the same order as the scale of hydrodynamic physically infinitesimal scale for gas. The infinitesimal scale for gas, in its turn is about the following order: $r_h = l/\sqrt{Kn}$, where l is the length of free pass of gas molecules, and Kn - Knudsen number. There is the possibility of studying the interaction between microfluctuations and usual hydrodynamic fluctuations.

5. Boltzmann Equation. Dynamics and Irreversibility.

The central point of the Boltzmann kinetic theory was H-theorem. The H-function is closely connected with the entropy of system, which was introduced by Boltzmann's immortal formula

$$S = k \ln f . \qquad (4)$$

L. Boltzmann showed, that the average entropy value (4), where the distribution function satisfies the equation (1), always grows or remains constant. The latter is possible only in equilibrium state. The second law of thermodynamics was proved by these facts, following the analyses of the molecule gas mechanics. It made the conflict between the reversibility of equations of motion in mechanics and irreversibility of thermodynamic system the point of numerous discussions, which have been going on till our days.

This discussion became especially acute after the Boltzmann's friend, I. Loschmidt remark, which was named the paradox of irreversibility, then after E. Zermelo's work, which was known as the paradox of recovery. The first of the paradoxes consists in the fact, that, if time is reversed at the moment $t_1 > t_0$, the system will change from more equilibrium state to non-equilibrium state due to reversibility of equations of mechanics. This fact contradicts H-theorem. E. Zermelo paradox is based on a well-known theorem about quasi-periodicity of Hamilton system movement. L. Boltzmann's objections were rather emotional. His two winged-word phrases are known to concern these paradoxes. The first one was, when he said: "Go and turn them (molecules)", the second one was: "You have to be waiting for a long time".

The irreversibility of the evolution of rarefied gas entropy is due to the irreversible properties of the equation (1), which is not invariant in regard to time inversion. The irreversibility of the equation (1) is considered related to the use of the condition of molecular chaos by its derivation. However, this point needs greater accuracy. Of cause, the use of any conditions of attenuation of the initial correlation brings to the irreversible equation because of the loss of some information. But in this case the condition of the molecular chaos is not the only reason of the irreversibility of the kinetic equation and not the most important one. If the pair distribution function is not supposed to be multiplicative, the kinetic equation will not be closed, but irreversible

$$\frac{\partial f_1}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_1}{\partial \mathbf{r}_1} = \int d\mathbf{v}_2 d\Omega v_{21} \left[f_2\left(\mathbf{v}_1', \mathbf{v}_2'\right) - f_2\left(\mathbf{v}_1, \mathbf{v}_2\right) \right]. \qquad (5)$$

The irreversibility is due to the time reading of the beginning and finishing of the act of two particles interaction. Consequently, the irreversible kinetic equations can be derived without the conditions of attenuation of the initial correlations. As an example of such equation one can take the master kinetic equation for rarefied gas [14].

What is the nature of the irreversibility and how can it be related to equations of mechanics? For a long time the first question of the two was traditionally answered as follows: the observed irreversibility is related to some incompleteness of the system description. In particular, when we study a system with a large number of particles, we always have to change level of description from a detailed dynamical one to some rough one. In this change some part of the information about the evolution of the system is being lost. Thus the irreversibility is related to the loss of some part of the information about the slate of the system. Such viewpoint became especially popular after the famous article of P. and T. Ehrenfest. This viewpoint was transformed as years were passing. During some lust decades the investigations decades in the sphere of theory of dynamic systems influenced this viewpoint essentially. The reversibility and determinism of the Hamilton equations solutions, describing dynamics of N particles, are known to be possible only at absolutely exact specification of the initial conditions. The considered systems with a large number of particles are very unstable dynamic systems. The more so, the movement in phase space is the movement with mixing in all real systems. Consequently, whatever small perturbations of the initial conditions lead to whatever strong deviation of the phase trajectory from its non-agitated state. So, it is clear, that specifying the initial conditions for a dynamic system with how ever small error, we make its evolution irreversible. A consistent rendering of this point of view can be found in a monograph of G.M. Zaslavsky [15].

Subjectivism of this explanation causes dissatisfaction. That is why another position is widely spread today, that relates the evident irreversibility to the quasi-open character of any physical system (see, for example, [16]). If to take into account the fact, that at presence of gravity field, system N of interacting particles cannot be considered as a closed one, then it is difficult to object to such explanation. The more so, closed systems are rather good models of really existing sys-

tems. But L. Boltzmann studied closed dynamical system, so the latter explanation can hardly solve the classical paradoxes. This contradiction leads to a number of serious difficulties in statistical mechanics. Perhaps one of the most explicit examples is the fact, that the molecular system coefficients of transport processes become zero, the coefficients are defined by Green-Kubo formulas. These formulas are strictly equal zero, due to quasi-periodicity of the closed system movement. Nevertheless they are widely used in molecular dynamic calculations, and give excellent results.

Perhaps the final solution of the conflict between mechanics and thermodynamics should be sought in refusing some idealizations of classic mechanics. We think, such idealization is the process of molecular interaction, which hardly can be described with the help of potential force.

6. Last Years

...Moving to Vienna in 1894 was certainly a mistake. Where is the dear to heart atmosphere of Institute of Physics? After Stefan had left, the Institute became alien. I do not understand its fussy workers, and I feel dull at the seminars. It is really true; one cannot enter the same river twice.

...Vienna seems to me cold. I think about Graz all the time. Henriett and girls loved it so mach. Today I was recollecting the farewell party, which I gave before leaving for Munich. There were many toasts and much music. I was loved there.

... Yesterday at the seminar I encountered with Mach again. The auditorium was full. "I won't permit to issue any article, if it contains elements, which cannot be observed experimentally. Nobody needs built on sand theories, even if one finds them witty. Physics is an experimental science, and not the place for philosophical reasoning, enveloped in mathematical form. Such reasoning is worth scholasticism. I appreciate professor L. Boltzmann as an experimenter, and his mathematical exercises are strange to me. It is remarkable, that even his friend, professor Loschmidt, who is occupied with an odd counting of non-existing atoms of the air, still has not accepted the notorious H-theorem". As a result I was in a temper, interrupted Mach with retorts, but did not say anything convincing. I am awfully tired of those fruit-

less discussions. How can not they understand, that the molecular-kinetic ideas not only give a new viewpoint on thermodynamics, but also a new method of nature's description and understanding.

...Yesterday at a sitting of the chemistry and physics society I delivered a speech, devoted to the memory of Iozeph (Loschmidt). I could not but say about his paradox: "This idea has not changed the word radically, but it has been still storming brains of numerous physicist-theorists. Reversibility, reversibility... Where did you see that reversibility?

...On the 5th of November Loschmidt memorial was opened. I was delivering a speech again. Certainly, significance of his last works far exceeds the boundaries of gas theory. The experimental proofs of atoms existence have been already acquired, and many times. It does not permit to doubt their real existence, and it does not depend on whether we can observe them directly or not. Only narrow-minded people, or people, who limited their opportunities with a wrong life position, can believe in existence of what they can only feel. Such position, turning into stereotypes, becomes the cause of sluggishness and dogmatism. It is sad, that those stereotypes are so popular among physicists. I can hear often, that mathematical physics is much more harmful, than alchemy, because it looks like science and stuffs students' heads with its useless ideas. Tell me, please, who doubts correctness of the calculation of the distance to Sirius, though none of the mortals ever measured the distance to this star with a tape measure.

... Leipzig met me with rain and railway station noise. I had not been here for a long time and forgot how the station fuss got on my nerves. Next day I went to Thomaskirche, and spent two hours sitting and listening to organ. Its music had always been comforting me when I went out, night had already put down its veil on Markt, and only lamps, like stars, had an attraction. People like moths moved from one lamp to another, disappearing on their way.

...Of cause, experiment is the source of our knowledge, but the knowledge becomes scientific, when it is systematized by a theory. And a direct description of a vast group of facts seems impossible here, what is possible is the mental image of the group. So we cannot say, like V. Ostwald: you should not imagine anything. We can only

say: you should add as little arbitrary features to your images as possible.

...Time derivatives demand that time in nature should be mentally divided into very small finite parts (time atoms). If I omit as not-proven by experiment, the notion, that deviation from the limit, approached by the image at getting smaller time atoms, I should accept, that the mechanics laws of a material point are correct only approximately.

...The notion of atoms as material points, and of forces as functions of distances between them, is provisional, but it should be preserved temporarily as we do not have a better one.

...If the mechanical explanation of nature is understood as based on the laws of modern mechanics, we should acknowledge as doubtful the fact, that future atomistic will become the mechanical explanation of nature.

...Yes, everything is alien to me here. Even students seem to me wooden idols, which can only understand the "Shun!" command and who are deprived of any fantasy. Spirit of Prussia is felt in Leipzig? Who might imagine that! My great grandfather lived in Kenigsberg, my grandfather – in Berlin, and my father left for Vienna. I took after my mother, who was Austrian. People breathe different air in Berlin and in Zaltzburg. One should not change the air, he breathed in childhood, and otherwise one won't avoid illnesses. That's why I suffer asthma. I must go back to Vienna. I am waited there; nobody has held the chair.

...Here is Vienna at last. I delivered an opening lecture. Mechanics became the leader in all physics today. Acoustics was the first to obey it, naturally and implicitly. The same thing happened with optics. The thermal theory was conquered by mechanics on the ground of the notion, that heat is movement of molecules. This conquest was possible, because the described hypothesis gives a very clear picture. We can explain mechanistically even the concepts of beauty and truth. Thus the almighty mechanics dominates both in nature and art, it also dominates in politics and in social life. God, on whose favor kings reign, is the main law of mechanics.

The task of the science is to explain complicated things through simpler ones. That's why physicists tend to explain the phenomena

like sound, light, heat, magnetism and electricity, reducing them to the phenomenon of the movement of small particles of bodies – molecules.

...We had to leave Ida in Leipzig to finish grammar school.

...Yesterday at the Academy sitting we discussed with excitement the significance of the atomistic theory. Suddenly Mach noticed sharply: "I don't believe the existence of atoms". All became silent; I was at a loss too. Then I reflected for a long time. Today the existence of atoms is no longer the matter of belief, neither the matter of convenient way of description.

...Suddenly the budget of my chairs turned out to be extremely insufficient, as the university had not given me what I expected to get.

...It's asthma, asthma. Nights are especially awful. I choke, and the darkness sucks me in, my breast is torn, my head is full of splitting noise. No other thoughts come to my mind, except for "I must breath". And I feel fear. God measures a term for everyone and gives a signs. I cannot but notice the signs.

...Unfortunately, the climate of California is not as pleasant as I expected. Subtropical heat and humidity, sudden changes from extreme dryness to fogs are too bad experience for a European to come through. I should add that I can't bear the local water; it upsets my stomach.

...Now atomistic can be considered as practically proved. Heat is certain to be connected with the movement of molecules. H-theorem is evident for me. But still there are damned questions, which I cannot answer. And I don't have strength.

Dumm ist mein Kopf und schwer wie Blei,
die Tobaksdose ledig,
mein Magen leer - der Himmel sei
dem Trauerspiele gnädig.

What's there further in the Schiller's rhyme?

Ich kratze mit dem Federkiel
auf den gewalkten Lumpen;
wer kann Empfindung und Gef ühl
aus hohlem Herzen pumpen?

Feur soll ich gießen aufs Papier
mit angef rornem Finger? --
O Phöbus, hassest du Geschmier,
so wärm auch deine Sänger.

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GENERALIZED BOLTZMANN KINETIC THEORY IN PHYSICS OF NEUTRAL AND IONIZED GASES

Alexeev B.V.
Lomonosov Academy of Fine Chemical Technology.

The classical Boltzmann equation is only valid on characteristic scales associated with the hydrodynamic time of flow and mean time between particle collisions. I have established (see, for example, [1]) that the inclusion of the third possible scale, τ, the time of particle collision, leads to the appearance of additional terms in the Boltzmann equation, which, generally speaking, are of the same order as the other terms in the Boltzmann equation. The generalized Boltzmann equation (GBE) for multycomponent mixture of reacting gases can be written in the form

$$\frac{Df_\alpha}{Dt} - \frac{D}{Dt}\left(\tau_\alpha \frac{Df_\alpha}{Dt}\right) = J_\alpha^{st,el} + J_\alpha^{st,r}, \qquad \alpha = 1,\ldots,\mu, \qquad (1)$$

where f_α - one particle distribution function for α- species; τ_α – mean time *between* collisions for α- particles; $J_\alpha^{st,et}$, $J_\alpha^{st,r}$ – Boltzmann collisions integrals for elastic and non-elastic collisions, *D/Dt* – substance derivative, containing generally speaking the self-consistent forces. It can be shown, that all known methods of the kinetic equation's derivation lead to GBE. In 1987 equation (1) was derived by the method of many scales. But to equation (1) lead the iterative methods of the kinetic equation derivation and the theory of correlation functions. In the theory of correlation functions the additional term corresponds to the local differential approximation of the non-local time-delay collision integral. It is shown that in the theory of plasma τ_α is mean time of the short distance collisions. In the kinetic theory of liquids τ corresponds the mean time of particle residence in the Frenkel cell. The through approximation for τ in rarefied neutral gas, plasma and liquid is delivered.

The GBE naturally leads, to a variation of the results in the sphere of traditional applications of the Boltzmann equation and to new hydrodynamic theory, which follows from the kinetic theory [1]. The following problems are considered on the GBE basement: structures of shock waves, propagation and decay of sound in perfect gas, strict theory of turbulent flows and its applications, generalized hydrodynamic equations for plasma, the charged particle distribution function in Lorentz gas, Landau damping in plasma physics, the transport processes in non- degenerated semi-conductors. It is shown, that the theoretical results based on GBE are in the good coincidence with the experiments even for the situations, in which classical theory leads to a difficulties. For GBE the generalized H-theorem is proved in 1992.

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PADE-APPROXIMATIONS IN THE KNUDSEN LAYER

Anolik M.V., Barantsev R.G.
Sankt-Peterburg State University

The problem of transition layers in asymptotical methodology can be solved in different ways. There are special functions connecting different asimptotics in one knot; the procedure of splicing of the expansion with regions of overlap is developed; the splicing of these two different asimptotics with the help of Pade approximation is in practices. The overlapping of regions is usually achived due to the complication of the internal asimptotics in the transition zone. Outside the transition zone the asimptotics remain simple, but regions of their application are separated with a transition layer. In such situation it is possible to build Pade-bridge, based on the simple asimptotics and connecting them.

The method of simple asimptotics connection is demonstrated with the example of Knudsen layer in monoatomic gas.

NUMERICAL UNSTABLE SOLUTIONS OF THE BOLTZMAN EQUATION AT SMALL KNUDSEN NUMBERS

Aristov V.V.
Computing Centre of RAS, aristov@ccas.ru

The fluctuations which have been observed in numerical solutions of the Boltzmann equation in problems for small Knudsen numbers (see [1]) by consideration of free jet flows are studied. Their possible relation to the description and modeling of turbulence in a gas is discussed. Numerical schemes are examined within the framework of the conservative splitting method on the basis of which instability in the supercritical regime is revealed. One can conclude that the explicit-implicit scheme can be used for stable stationary solutions and for unstable unstationary solutions (for flows which are stationary at averaging on large time scales). In unstable flows the time step can exceed a kinetic time scale as the characteristic scale of turbulent fluctuations (that shows also comparison with experience), essentially exceeds a characteristic kinetic time. The instability and the nonequilibrium results in the substantial growth of the transfer of momentum and heat, i.e. the growth of values of nonequilibrium stress and of heat. In this fact the basic hypothesis is consisted about an importance of the use of the Boltzmann equation for the description of turbulence. It is supposed, that at instability a character of the distribution function becomes non-stationary and nonequilibrium. For studying numerical solutions the unstable pulsation of density is analyzed and comparison with the available experimental data for turbulent jet flows is made. The influence on fluctuations of the reduction of a value of the time step is investigated. At essential the reduction of this parameter down to kinetic scale a character of pulsation essentially was not changed. The change of magnitudes of amplitudes of fluctuations of density, viscous stress and heat flux is less than a scale of the amplitude itself. The difference of behaviour of the nonequilibrium dissipation from the Chapman-Enskog description is noted. In the present paper an attempt of the comparison of the schemes with known simple nonlinear models of iterations describing the phenomenon of the deterministic chaos is made.

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DEVELOPMENT OF THE DETERMINISTIC METHOD FOR SOLVING THE BOLTZMANN EQUATION

Aristov V.V., Zabelok S.A.
Computing Center of RAS, aristov@ccas.ru

Recently several numerical methods of solving the Boltzmann equation with the deterministic (without Monte Carlo procedure) evaluation of the collision operator were suggested. In the deterministic approach [1, 2], used in the present paper, the exact integration over impact angles is carried out. Molecular models for which a semi-analytical method is directly applicable are studied. The formal

scheme of the finite element method in velocity space is used. There are advantages of this approach in comparison with more widespread probabilistic (Monte Carlo) methods. The collision term in the right hand side is approximated by the quadratic form with constant coefficients, that makes clearer the non-linear structure of the integral (a disadvantage of the approach is a large number of elements of a matrix of the quadratic form). As a result of partially analytical calculation there are new algorithmic opportunities. The number of numerical parameters is small: in the homogeneous isotropic relaxation problem this number equals to three, for a one-dimensional stationary problem -- to four. With this method being used it is possible to obtain tests with the fixed accuracy for simple problems. This important feature (small number of parameters) makes the algorithm quite simple for multi-dimensional problems. Schemes are well paralellized in velocity space, that allows us to apply effectively enough them in calculations on modern supercomputers. Solutions for relaxation problems with the fixed accuracy are obtained, comparison with the solution by other regular method [3] for a one-dimensional heat transfer problem is made, various two-dimentional problems are solved, three-dimensional jet flows are studied.

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METHODOLOGICAL STATUS OF ASYMPTOTICS

Barantsev R.G.
Sankt-Peterburg State University

Asimptotical methods are meant for simplifying problems and their solutions near singularities, the accuracy of the methods is increasing as they approach the singularity. But the accuracy of the asymptotical solution in a given region is always

limited. For a long time this inherent inaccuracy made us reber the asymptotical methods rather to art then to science.

Howerer the requirement of ultimate accuracy, pertinent in reference to models, is excessive in reference to real objects. In a new paradigm the former disadvantage of the asymptotical methods turns into an advantage.

In the report the fundamental essence of asimptology and its role for providing the relationship between analytical and numerical methods is discussed.

NUMERICAL AND EXPERIMENTAL INVESTIGATIONS IN THE RARIFIED GAS DYNAMICS AND THEIR APPLIANCE IN SPACE-ROCKET ENGINEERING

Bass V.P.
Institute of Technical Mechanics of The Ukrainian Science Academy and National Space Agency of the Ukraine, bass@pvv.dp.ua

From the first days of the exploration of cosmic space the molecular kinetic theory became the general foundation, which gave the basis for stating the laws of flow past spacecrafts (SC) with a flow of rarefied gas, and the basis for studying various physical processes in this sphere.

The methods of rarefied gas dynamics and molecular gas dynamics have found series of modern applications in the development and operation of the objects of space engineering. The present report gives a short review of the main results of numerical and experimental investigations, obtained by the body of scientists of the department "Rarefied Gas Dynamics" of the Institute of Technical Mechanics of The Ukrainian Science Academy and National Space Agency of the Ukraine for the last 30 years. The subjects of our department embrace the following main trends:

1. development and foundation of numerical methods, algorithms and software tools for conducting investigations of aerodynamic, thermal characteristics and processes of mass transporting in the neighborhood of orbital and descent modules;

2. aerodynamic modeling of the flight conditions, experimental investigation of the interaction peculiarities of the supersonic neutral rarefied gas flows and the flown surface, as well as the conduction of complex tests and calibration of the aircraft measuring systems and devices;
3. development of concepts, formulation and realization of space scientific and applied experiments.

Physical analogy of the molecular transportation and radiation transfer processes in vacuum made it possible to adapt the available mathematical and software tools in appliance to the solving of modern tasks of space ballistics, geodynamics, satellite photometry, irradiative heat exchange, and others. The presented results of their solving show the strength and effectiveness of the tools of the molecular-kinetic gas theory, which basis was founded by Maxwell and Boltzmann in the previous century.

THE DISTRIBUTION FUNCTION FOR A SUBSYSTEM EXPERIENCING TEMPERATURE FLUCTUATIONS

Bashkirov A.G.
Institute Dynamics of Geospheres, RAS, abas@idg.chph.ras.ru

The Renyi entropy with a free Renyi parameter q is the most justified form of information entropy, and the Tsallis entropy may be regarded as a linear approximation to the Renyi entropy when $q \approx 1$. When $q \to 1$, both entropies go to the Boltzmann--Shannon entropy. The application of the principle of maximum of information entropy (MEP) to the Renyi entropy gives rise to the Levy distribution (or, q--distribution) accepted as one of the main results of the so-called non-extensive statistics. The same distribution is derived here for a small physical system experiencing temperature fluctuations. The long-range "tail" of the Levy distribution is the power-law distribution with the exponent s expressed via q. The free Renyi parameter q can be uniquely determined with the use of a further extension of MEP. Then for the exponent s, the values are found within the range of typical values, $1.5 \div 2$ in dependence on parameters of stochastic systems.

INFLUENCE ON COLLECTIVE INTERACTION EFFECTS WITH A CARRYING MEDIUM TO THE NANOPARTICLES DIFFUSION

BelkinA.A., Rudyak V.Ya.
Novosibirsk State University of Architecture and Civil Engineering,
rudyak@ngasu.nsk.su

Wide application and the unique properties of materials cause increasing interest to a problem of the description of transport processes, passing in dispersed nanosystems. Today it is already clear, that the mechanisms of these processes are specific and are not featured by the known theories. For their investigation and calculation of transfer coefficients it is necessary to research qualitatively and quantitatively dynamic effects of nanoparticles interaction with a carrying medium. The direct numerical simulation is an irreplaceable tool in such researches today. Numerical calculations [1,2], fulfilled by a molecular dynamics method, have shown, that the velocity autocorrelation function of nanoparticles has two parts of relaxation. First of them is connected with individual nanoparticles interactions with a carrying medium molecules and is well investigated. It cannot be said about the second area of relaxation, which in some situations brings in the main contribution to a diffusion coefficient. The present paper is devoted to research of its nature.

Nanoparticle and the molecules of an environment were simulated by absolutely hard spheres of various radius and mass ($R/r = 4{,}5$, $M/m = 50 \div 200$). Density of a carrying medium also varied. Fluids, dense and moderately dense gases were investigated. The "particle — molecules" velocity correlation functions are calculated. The calculations have allowed to fix sound waves raised by a moved particle in a carrying medium, and to measure speed of their distribution. Most interesting is the detected for the first time second maxima of the correlation function. Its value exceeds value of the first, "sound" maxima for massive nanoparticles. The correlation, appropriate to it, is long-lived (more than twenty mean free times).

Thus, the driving nanoparticles generates collective fluctuation of impulse of a carrying medium. The interaction with this fluctuation generates the second exponential area of particles relaxation. It is es-

sential, that the influence of fluctuations on nanoparticles motion is delaying, the instantaneous velocity correlations are peer to zero.

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PHORETIC PHENOMENA IN AEROSOLS: THE GAS-KINETIC ANALYSIS AND COMPARISON WITH EXPERIMENT

Beresnev S.A., Chernyak V.G.
Ural State University, Ekaterinburg,
Sergey.Beresnev@usu.ru, Vladimir.Chernyak@usu.ru

The brief review of the theoretical results for phoretic phenomena in aerosols (thermo-, photo- and diffusiophoresis; drag force) obtained by the authors in the last years is presented. Within the framework of a single particle in unbounded gas model by using of the adequate gas-kinetic model equations (the S-model for monatomic gas and the McCormack model for a binary gas mixture) the linear boundary problems for phoretic forces and velocities of a spherical particle are formulated and decided. In all cases the integral-moment method for the solution of gas-kinetic equation to describe the problems at arbitrary Knudsen numbers is used. The closed system of integral equations is solved by a Bubnov-Galerkin method with the justified choice of trial functions. In boundary conditions for a velocity distribution function the opportunity of an arbitrary accommodation of tangential and normal moments and energies of gas molecules on the particle surface is allowed by introduction phenomenological Knudsen accommodation coefficients.

The results of the problem solution are the values of phoretic forces and particle stationary velocities depending on Knudsen number and other defining parameters (accommodational, thermal and optical properties of gas-particle system). In limiting on Knudsen number regimes (the viscous-slip and the free-molecular regimes) by asymptotic expansions of Galerkin coefficients the analytical expressions for phoretic forces and velocities are obtained. With the purpose of practical usage of obtained results the analytical expressions fitted gas-kinetic calculations in wide range of Knudsen numbers with error no more than 3 % are offered.

The comparison of the obtained data with theoretical results on the basis of linearized Boltzmann equation (Sone et al. and Loyalka et al.) the good agreement is exhibited. The theoretical results are compared in detail with the most reliable experimental data. The problems of further development of theory (in particular, deposition of aerosol particles from non-equilibrium gas on the surfaces) are considered. The feasibility of the obtained results for the analysis of appearances in the upper atmosphere (photophoretic levitation of particles in the stratosphere and mesosphere) is discussed.

SIMULATION OF PROCESSES RAREFIED PLASMA FLOWING OUT AT THE ELECTRIC THRUSTER

Bishaev A. M., Kim V.
RIAME MAI, riame@sokol.ru,

Nowadays the electrical thrusters application in space technology is extended significantly. Analysis of the characteristic sizes and density number of interacting plasma component in plume of the stationary plasma thruster (SPT) shows, that all Knudsen numbers are great enough (at least, for distances of 20-30 calibres from the thruster exit), what confirms about the necessity of the plasms movement description at kinetic level. In the paper [1] on the basis of modelling Hamel kinetic equations for a mixture of ions and neutrals under assumption of axial symmetry the problem statement for the plume plasma dynamics discription is considered. In contrary to similar tasks of rarefied gas dynamics in kinetic equation for ions there is a member tak-

ing into account the electrical field impact on their movement. Electric potential is determined from the equation of electron movement with usage of severel assumptions (see [2]). In [1] the numerical method of the mentioned problem solution was obtained which reproduced the basic features of the SPT plume known from experiments (presence of the back ion flows and appearance of area of increased density of ions called "crossover" at the axis of symmetry). In [3] therewas constructed the kinetic model (type of Krook model), which took into account a resonant charge-exchange collisions-special type of interaction of ions and neutrals, This interaction has the greatest cross section area. Use of new model had given appreciable increase of back ion flow currents. Further on the basis of the mentioned above model there was created computing complex "Jet", giving acceptable correspondence simulation and results experimental measurements. Results of this comparison are given in [4]. In the given report the three-dimensional problem statement for SPT plume considered to take into account impact of back flows on thruster and spacecraft. To solve this problem the new numerical method is used.

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DUAL VARIATIONAL PRINCIPLES THE LINEAR BOLTZMANN EQUATION

Bishaev A.M., Rykov V. A.
RIAME MAI, Computing Centre RAS riame@sokol.ru,

In papers [1], [2] for the linear stationary Boltzmann equation there were constructed two minimax variational principles. First of them [1] is based on the description of a gas with the help of an even part of distribution function and macroscopic components of speed. The second variational principle [2] is based on an odd part of distribution function, pressure and temperature of the gas. The extreme meanings functionals of these variational principles are equal to capacity of force of resistance of a body in a task of slow (Stokes) flow of rarefied gas . The variational principles are an effective means for calculating of extreme meaning of functional, as the mistake by order ε in trial function causes to a deviation functional from its extreme meaning by order ε^2. The greatest success in calculating with a variational method is obtained, when it is possible to construct two variational principles, which extreme meanings are equal to seek value. One of the functionals is a minimum principle, and another is a maximum principle. The calculating of functionals with the help of the coordinated trial functions gives the approximated meaning of seek value with overmuch and with lack. Average value of these functionales refines the results, because a deviation functionals from exact value are distributed opposite and basically compensate each other. In [3] variational principles are applied to calculating of sliding factor, which is equal to the minimal meaning of functional of a variational principle [1] and maximal meaning of functional of a variational principle [2]. It's shown in this report , that generally, under some conditions on sets of varied functions, variational principle [1] is a principle of a maximum, and variational principle [2] is a principle of a minimum. Calculating the resistance of the heat-conducting sphere is given as an example of using dual principles at any Knudsen numbers.

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INVESTIGATION OF THE STRUCTURE OF THE SHOCK WAVE FRONT IN THE ATMOSPHERE OF MARS

Bondar E.A., Gimel'shein S.F., Markelov G.N., Ivanov M.S.
Institute of Theoretical and Applied Mechanics, bond@itam.nsc.ru

The history of cosmonautics counts more than 30 launches of spacecrafts to Mars, and some more launches have been planned for the future decade. Successful maneuvering in the atmosphere of Mars demands detailed knowledge of physical processes in the flow past spacecraft at different altitudes. For acquiring true information about peculiarities of the flow it is necessary to use the numeric simulation, which not only completes experimental investigation, but is the only source of data at the study of such flow conditions, which make it difficult to use any ground experimental facilities.

Method of direct statistical simulation proved to be good for the chemically active N_2-O_2 flows, surrounding bodies, coming into the Earth atmosphere. The correct accounting of real gas effects is known to be necessary for simulating such flows (excitation of inner degrees of freedom and chemical reactions). This very feature is a key feature for simulation of CO_2-N_2 flows around the bodies in the atmosphere of Mars. It should be noticed, that the description of chemical reactions and energy transfer between the translational and internal modes for the mixture of CO_2 and N_2 in the direct statistical simulation method is a difficult task. It is due to the fact, that at present there is no generally accepted collisions model for polyatomic molecules, such as CO_2.

The main purpose of the present work is the numeric investigation of the structure of the shock wave front near the body, entering into the atmosphere of Mars whith the help of the method of the direct statistical simulation, using various models of descriptions of the real gas effects. The following key points were considered in this work:

1. *Influence of the effect of rarefaction.* The structure of the leading shock wave front near the cylinder with the radius of 1 m has been studied in the Knudsen number range from 0.001 to 0.01.
2. *Influence of the description models of the real gas effects.* The results have been received for various models of the internal degrees of freedom (comparison of the continual and discrete approaches have been done). The influence of chemical reactions on the structure of the wave front has been investigated. Verification of a new discrete model of the chemical reaction description in the method of the direct statistical simulation has been done.
3. *Distribution functions.* Non-equilibrium inside the shock wave front has been studied on the level of distribution functions of translational, rotational and vibrational energy.

NUMERIC SIMULATION OF THE STATIONARY PLASMA ENGINE JET

Bondar E.A., Shweigert V.A., Ivanov M.S.
Institute of Theoretical and Applied Mechanics, bond@itam.nsc.ru

Stationary plasma engines (SPE) – belong to one group of electrojet engines, used for the orientation control and for the correction of the orbital stations and satellites trajectories. At present the question of the degree of shortening of spacecrafts service life because of the interaction of SPE engine jets and the sensitive spacecrafts construction units remains open. The main components of this interaction are:

- bombing of the surface with the quick ions of the working substance (which is xenon, as a rule), the bombing is possible because of the big angular divergence of a jet (up to 60^0)
- and reverse flow of the slow ions on to the surface, the slow ions appear in the process of the resonant charge exchange of the quick ions on the atoms of non-ionized working substance.

The surface sputtering intensity depends on both material properties and local characteristics of the jet, such as flow density of the falling ions and their energy distribution and angle of incidence distribu-

tion. These parameters are well described with a simple semi-empirical model in the central part of the jet, formed by the quick ionic flow. The description of the reverse flow of the slow ions is an essentially more difficult task. In particular, the results of measurements, conducted in vacuum chambers are not suitable for the evaluation of the parameters in the sphere of the reverse flow of the jet, flowing into space (first of all, it is connected with the influence of the residual gas on the structure of the jet in the chamber).

In present work the structure of the jet of the stationary plasma engine is investigated numerically with the employment of the method of particles (Particle-in-Cell / Monte Carlo collisions). Verification of the approach is fulfilled on the ground of comparison of the simulation results of jet, flowing into a vacuum chamber (taking into consideration the influence of residual gas) and the experimental data. Good accordance has been found both in total ionic current and in the ionic current density profile at various distances from the engine outlet.

The important result of the simulation of the stationary plasma engine jet effluence into the cosmic space vacuum is rather high-acquired value of the energy of slow ions in the area of reverse flow (about 70 eV). Appliance of the model, taking into account inhomogencity of the electron temperature in the jet, for the calculations brings to a still higher value of the slow electron energy (up to 100 eV).

ON POSSIBLE FRACTAL STRUCTURE OF THE TENSOR OF TURBULENT DIFFUSION COEFFICIENTS IN ATMOSPHERIC BOUNDARY LAYER

Borodulin A.I.
GNC «Vector», borodulin@vector.nsc.ru

The results of experimental determination of the tensor components of the turbulent diffusion coefficients obtained in the atmospheric boundary layer during a four-day observational period are considered. Besides a clearly pronounced diurnal, almost repetitive, variations of its components, considerable oscillations, which can't be explained by the presence of measurement errors, are revealed. An attempt to explain such a behavior of the tensor components of the turbulent diffusion coefficients by fractal structure of the observed process is made in this presentation.

MODELS OF PULSED LASER ABLATION

Bulgakova N.M., Bulgakov A.V.
Institute of Thermophysics SB RAS, nbul@itp.nsc.ru

The range of applications of Pulsed Laser Ablation (PLA) is continuously expanding. The application list, far from being complete, includes laser welding, cutting, drilling, cleaning, and structuring of solid surfaces, thin film deposition, synthesis of new materials, manufacturing of microdevices, chemical analysis of substances, various applications in medicine. In view of a variety of physical and chemical processes, which take place in the PLA, the description of this phenomenon requires a combination of different fields of knowledge. In most applications, optimal laser irradiation regimes have been found by empiric ways only. Thorough investigation and modeling are necessary for optimization of PLA in the existing applications and for elucidation of new utilization possibilities.

In this work we present a number of models developed for the description of the laser plume dynamics under the different conditions of solid target irradiation. The first model describes the dynamics of a quasi-stationary laser plume formed under the action of millisecond laser pulse. The general features of pressure pulsations on a solid surface are considered. It is shown that two fundamentally different laser plume structures are developed, depending on the irradiation conditions.

The second model is a gas dynamic spherical model describing expansion of material vaporized by a nanosecond laser pulse from a flat surface in an ambient gas. The model describes in details the gas dynamic behavior of the laser plume for the actual experimental conditions, including the plume pulsations. It is found that the ionization/recombination processes play an important role in the formation of the gas dynamic parameters of the expanding plasma.

For the non-spherical laser plume, a new approach to the analysis of the expansion dynamics is proposed. The approach is based on the analogy with a stationary gas jet issuing from a sonic nozzle into an ambient gas. With the help of this analogy, the experimentally observed phenomenon of the laser plume focusing is explained. It is shown that the plume formation is accompanied by the vortex structure development at the plume periphery.

To describe the PLA in vacuum, the concept of a double layer is employed. It is shown that the fast ion generation observed in many experiments is caused by the high-energy electrons generated in the plume due to the laser radiation absorption in plasma, which cannot be described in the frames of a single-temperature electron distribution function.

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NUMERIC INVESTIGATION OF HIGH-ALTITUDE AERODYNAMICS OF "EXPERT" CAPSULE.

Vaschenkov P.V., Ivanov M.S.
Institute of Theoretical and Applied Mechanics of the Siberian Branch of Russian Academy of Science, vashen@itam.nsc.ru

At present time international research centers studying high atmospheric layers and the cosmic space are increasingly interested in descent modules for repeated use. Launching of comparatively inexpensive test modules is planned in accordance with the program European Experimental Reentry Testbed (EXPERT) to study the influence of atmosphere on space vehicles returning from the orbit and to investigate peculiarities of the gas flow near the vehicles.

The purpose of the program "EXPERT" is to succeed in getting lower cost of the experiments with the descend modules, to investigate the peculiarities of hypersonic flows, such as transition of a boundary layer into a shock layer, flow separation, the interaction between the shock wave and boundary layer.

In present work altitude aerodynamics (H > 75 km) is being studied for returnable capsules. of 3 types: with a pointed spherical

nose and conical body, "wave" type capsule with a blunt nose and cylindrical body and the "KHEOPS" capsule, which is a pyramid with an elliptical nose and rounded faces. The distributed aerodynamic characteristics, such as thermal flow, drag coefficient, pressure coefficient and others have been investigated alongside with the flow characteristics and integral properties of the capsules.

The flow of the capsule with the diatomic gas stream was studied. The excitation of rotational and vibrational degrees of freedom of molecules was taken into account in the calculations. The Knudsen number of the incident flow varied from a free molecular one to Kn = 0.001. Mach number of the flow equals M = 28. The flow near the capsule was calculated with the Monte Carlo direct statistical method. The collision number was calculated with the method of majorant frequency. Molecule collisions were calculated according to the model of variable hard spheres. Inner degrees of freedom were taken into account according to the Larsen-Borgnakke model. Axially symmetrical and three-dimensional variants of the program SMILE, created at the Institute of Theoretical and Applied Mechanics of the SB RAS,was used for the calculations.

The acquired results draw to a conclusion about advantages and disadvantages of each type of capsules from the viewpoint of aerodynamics. The data about the value of the heat-transfer coefficient along the surface may be used for designing the method and system of the capsule cooling.

NUMERIC SIMULATION OF HIGH-ALTITUDE AERODYNAMICS OF THE "PROGRESS" SPACECRAFT

Vaschenkov P.V.[1], Ivanov M.S.[1], Markelov G.N.[1], Kashkovskii A.V.[1], Krylov A.N.[2]
[1]- Institute of Theoretical and Applied Mechanics of the Siberian Branch of Russian Academy of Science, vashen@itam.nsc.ru
[2]- Rocket-Space Corporation "Energy", Andrey.N.Krylov@rsce.ru

The useful load (UL), launched into orbit, after the dropping of the streamlined nosing, undergoes the influence of the incident flow.

An earlier dropping of the streamlined nosing increases to some extent the launched mass of the UL, however bigger dynamic pressure (caused by denser atmosphere in the point of dropping) may result in the rise of thermal and force effect on the useful load. Reliable data about the character of the flow of the nose part of UL is necessary to determine the optimal altitude of the dropping of the streamlined nosing. At present the development of the numerical methods of the rarefied gas dynamics enables fulfillment of three-dimensional calculations near the complex form bodies. In the Rocket-Space Corporation "Energy" pressure measurements near the spacecraft "Progress" were conducted in flight after the dropping of the streamlined nosing. During information processing of the results of a natural experiment complex application of both numerical calculations and experimental data makes it possible to analyze profoundly all factors, influencing indications of sensing elements.

In present work the numeric simulation of the streamlined nosing flow of the spacecraft "Progress" with rarefied gas after dropping of the shutters of the streamlined nosing is carried out. Parameters of the incident flow correspond to the conditions of 76 km altitude; pressure 0.6 Pa, temperature 190 K, Knudsen number of the free stream Kn $\approx 2\ 10^{-3}$, the velocity of the stream 2.1 km/s. The simulated gas is nitrogen. Chemical reactions were not taken into consideration.

The simulation of the streamlined nosing flow of the spacecraft "Progress" was carried out in different configurations: a simplified model (without superstructures) which permits solving the task in axially symmetric formulation, and a full model (with superstructures), which demands three dimensional formulation of the problem. Influence of a small angle of attack on the aerodynamic characteristics of a body was also investigated.

The calculations were made with Monte Carlo direct statistical simulation method. The collision frequency was calculated with the majoritary frequency method. The molecule collisions were carried out according to the model of variable hard spheres. Internal degrees of freedom were taken into consideration according to the model of Larsen-Borgnakke. The axially symmetric and three dimensional variants of the SMILE program, created at the Institute of Theoretical and Applied Mechanics of SB RAS, were used for the calculation.

ONE-DIMENSIONAL BOLTZMANN EQUATION AND DISCRETE MODELS

Vedenyapin V.V., Amosov S.A., Adzhjiev S.Z.
Institute of applied mathematics of the Russian Academy of Science,
vicveden@keldysh.ru

In the report one-dimensional Boltzmann equation for a multicomponent mix of chemically inert gases is considered. This equation possesses one remarkable property – its collision integral includes only collisions between particles of different kinds. The contribution of homogeneous reactions to the collision integral is equal to zero as one-dimensional laws of conservation of a momentum and energy suppose only trivial solutions for particles of the same kind. In this case the momentums of colliding particles do not change.

The invariant functionals of the considered equation have been investigated. They correspond to the conservation of particles number of each kind, a total momentum and energy.

Also in the work the discrete models of Boltzmann equation are considered. One of them is the infinite model with discrete momentums in each integer point. The theorem of the weak approximation of solutions of the initial continual equations is proved by suggested discrete model.

Then the properties of the finite models, in which discrete momentums are located zero symmetrically, are studied. Here the main problem is the construction of the models possessing a set of invariants, corresponding to the set of the continual Boltzmann equations. The models with the correct invariants number are named exactly conservative or normal ones.

The problem of superfluous invariants of the discrete models has been resolved rather recently (details are represented in [1]) by the procedure of inductive construction of models with the calculation of the invariants number on each induction step. The elementary not trivial finite model for a two-component mixture is the seven-point model [2] for the ratio of weights equal 3. This model is the only one of not trivial finite one-dimensional models with the property of the exact conservatism, zero symmetric, known today.

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BEAM AND MOLECULAR DYNAMICS INVESTIGATIONS OF CLUSTERS FORMATION AND PROPERTIES

Vostrikov A.A., Dubov D.J., Drozdov S.V.
Institute of Thermophysics, vostrikov@itp.nsc.ru

In the report the following results of the molecular-beam and molecular-dynamic researches of the formation and properties of the clusters are submitted.

- The features of formation and growth of the molecular gases clusters in supersonic free jets [1]. Special attention is given to the influence of the gas vibrational nonequilibrium on an initial stage of condensation and to the formation of mixed clusters at the expansion of the molecular gas mixtures.
- The structure and energy parameters of the small water clusters, formed on the basis of the polarizing Stillinger model, in which the molecules of water are not "hard" and can experience ionic dissociation.
- The features of the collision of neutral and charged clusters with a solid surface [2]. The influence of the size and kinetic energy of the cluster, colliding with a surface, on the condensation, scattering indicatrixs and polar cluster ionization is considered. The characteristic features of the kinetics of the initial collision moment, in particular, the nonequilibrium character of the collision energy distribution inside the cluster, are established with the molecular dynamics method. The results of the beam measurements of the influence of the charged cluster size on the electron emission at the cluster collision with a metal target are submitted.

- The features of molecular clusters collision with one another, and also with an electron and a proton. Special attention is given to the results of the beam and molecular-dynamic researches of proton capture by water clusters in different collision processes. The dimensional effects of the electron attachment to clusters, the clusters ionization and the electron-induced luminescence of clusters are briefly considered. Conclusions about the mechanisms of energy dissipation of internal excitation in clusters of different types are made via comparison of the results of the interaction of the molecular clusters and the strong-bonded cluster C_{60} with an electron [3].

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EXACT SOLUTION OF THE BOLTZMANN-MAXWELL KINETIC EQUATION

Galkin V.S., Zharov V.A.
Central Aerohydrodynamic Institute

Maxwell's role in the derivation of the kinetic equation is considered. There is a review of exact solutions on the following points: local Maxwell solutions; spatial homogeneous relaxation of a binary mix; homoenergic affine flows; dominant and power solutions. New results are presented on the second and third points. The term "exact solutions" is used for the explicit solution of the kinetic Max-

well transport equation or equations solution by moments method, that is with the help of elementary and special functions.

SURFACE STRUCTURE SIMULATION IN GAS DYNAMICS WITH THE USE OF ATOMIC FORCE MICROSCOPY DATA

Gerasimova O.E., Borisov S.F.
The Ural State University, Ekaterinburg

As it is known, the problem of boundary conditions to gas dynamics tasks frequently rests on ignorance of real surface structure from which the gas molecules interact. At the same time, experiments show, that so-called surface "roughness" at a nuclear level and above influents significantly on energy and momentum exchange at internal and external gas flow. Therefore attempts to construct boundary conditions, including a surface ideally smooth, or consisting of the elementary structural identical elements, result in the inadequate description of gas scattering by a surface.

In connection with development last years methods of scanning probe microscopy, in particular, atomic force microscopy, there is an possibility of detailed studying specific features of surface structure and the account of these features at construction of boundary conditions.

In this study the attempt of surface structure simulation of silicon single crystal with the use of atomic force microscopy data is made. The samples, exposed to chemical etching and subsequent oxidation, have been investigated. Thus the surface structures with a various degree of a roughness which was estimated from topographical images were formed. As a result of research the data on a surface microstructure are obtained depending on a way of preparation and, in particular, from oxidation time after chemical cleaning during the interaction with atmospheric oxygen. The different parameters characterizing surface structure, in a particular, fractal dimension, average roughness value, root-mean square roughness have been determined.

For the description of surface microstructure the statistical model of cones suggested in work [1] was chosen. This model seems more adequate to the real situation. However, the next step has to be made

to improve it: to include in consideration cones' function distribution on the height. Such function of distribution of surface structural elements (cones) on heights was constructed on the data obtained from topogramms.

The research described in this publication was made possible in part by Awards CRDF No: REC-005 and INTAS No: 99-00749.

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SIMULATION OF DISPERSION OF METALLIC CLUSTERS AND MACROMOLECULES AT A SOLID SUBSTRATE BY THE METHOD OF MOLECULAR DYNAMICS

Golovnev I.F., Fomin V.M.
Institute of Theoretical and Applied Mechanics,
golovnev@itam.nsc.ru

Creation of a new generation of computers based on molecular film causes a range of problems on synthesis of molecular nanostructures with the properties preset at the substrate surfaces. The macromolecules of phthalozianine of metals consisting of 57 atoms are found more perspective for these aims. The problem of synthesis of copper contacts at the surface of molecular crystals is also important. One of the possible criterion is the method of a molecular-beam epitaxy, when the copper clusters are absorbed at dispersion by the surface. The problem of description of the phenomena in metallic clusters at collision with the substrate also occurs in technological problems of surface coatings, for example, in a cold gasdynamic spraying. The fact that in the both cases the dispersion of the system with a number of atoms having their interior structures is considered at the solid substrate surfaces, makes these problems common from the fundamental point of view.

To investigate these processes one uses a propagator realization of the method of molecular dynamics. The basis for this realization is an algebraic modification of classical mechanics, in which the basic

equations of dynamics have a form of evolution combinations, not the differential equation, as, for example, in Gamilton's mechanics. Within the framework of a propagatory mechanics we show the equivalence of the Gamilton pictures (the mechanics of discrete system of particles) and the Liouville's picture (the kinetic theory) that is one of the important advantage of such approach. The present work considers a collision of the spherical copper clusters in the velocity interval up to 1000 m/s at the structureless substrate simulating an absolutely rigid wall. Three intervals of the cluster initial velocities have been revealed that are fundamentally differed on the dissipation mechanism of kinetic energy of a gravity center: quasi-elastic, elasticoplastic, and strongly plastic; these processes have been physically analyzed. One demonstrates that at high velocities the cluster is melted at the contact.

The dispersion of molecules of the copper phthalozianine at the silicon substrate was numerically studied. The interior degrees of freedom of both molecules and substrate were taken into account. A strong effect of a molecule rotational energy on their absorption have been found. A phenomenon of a molecule self-organizing into a nanocrystal with a α-modification structure of a molecular crystal occurs at simulation of the dispersion of the molecule ensemble of the copper phthalozianine

GASDYNAMIC IMPACT ON NUCLEATION PROCESS

Gorbachev Yu.E.
Institute for High Performance Computing and
Information Systems. gorbachev@hm.csa.ru

One of the most perspective recent ideas for kinetic theory development is formulated in an approach to hydrodynamic equation derivation from kinetic ones [1-3]. In the framework of this approach hydrodynamic variables are considered to be slow in the sense of the singularly perturbed evolution equations theory, while the hydrodynamic equation derivation procedure consists in elimination of fast variables (Chepman-Enskog is one of the applications of the method).

Condensation process analysis shows the presence of its fast stage, namely nucleation one, during which the quasistationary cluster size distribution function formation takes place. However separation of fast and slow variables describing nucleation and condensation processes respectively is connected with large problems due to existence of a number of characteristic times. Cluster size distribution function evolution is determined by the kinetic relaxation time τ_k, as well as by series of partial time lags $\tau_d(g)$ of g-mer formation (clusters of g monomers) [4]. Time $\tau_d(g)$ increase with g, and $\tau_d(g) < \tau_k$ for $g < g_*$. As a sequence, the quasistationary distribution function formation for subcritical clusters is determined by kinetic time only, that makes the description of the system for such cluster sizes more simple. For $g > g_*$ one has the opposite relation for this characteristic times, and, starting from some cluster size g_M, $\tau_d(g)$ become equivalent to the hydrodynamic characteristic time τ_h, that means that the rather large clusters evolves at time scale τ_h only. Thus the brief description of condensation process demands some additional approaches, for instance, the condensation fraction concept engaging.

Starting from Zel'dovich equation it was shown that the slow evaluating part of the cluster size distribution function, that is the quasistationary distribution, depends not only on hydrodynamic (slow) variables, but on their time derivations also. For stage $(t - \tau_d) >> \tau_k$ the asymptotic expression for both quasistationary distribution function and for quasistationary g-mer's flux is obtained.

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EVALUATION OF THERMAL SLIP VELOCITY WITH USING OF THE KINETIC EQUATION OF BOLTZMANN-ALEXEEV TYPE

Dudko V.V., Yalamov Yu.I.
Moscow State Regional University, vladimi2000@mail.ru

B.V. Alexeev suggested the variant of Boltzmann equation. In this variant the changes of molecule's function of distribution take into account on the time similar to time of collision of molecules [1,2].

In this work the decision of task about the thermal slip of the heated up gas is nonuniform with using the equation of Boltzmann-Alexeev type and the dependence of coefficient of thermal slip from Π - coefficient of the correction term to the Boltzmann equation was received.

The gas fills in half-space limited to a wall. The gradient of temperature is directed along a surface of the wall. Outside of Knudsen's layer the velocity of gas is equal to velocity of thermal slip.

For integral of collisions the BGK-model is used. The equation of Boltzmann-Alexeev is solved by a method of the moments. The Maxwell boundary conditions and conditions, similar to them, for derivative function of distribution were used.

If value of parameter $\Pi=0$, factor of thermal slip $K(0) = 1,17$. This value is known [3] and corresponds to the Boltzmann equation. If value of parameter Π to increase, K will increase to 21.If value of parameter $\Pi=0.8$ [1], then $K(0.8)=15.67$.

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FORMATION OF NEUTRAL AND CHARGED CLUSTERS NEAR AIRPLANE IN ATMOSPHERE AND AT AERODYNAMIC MODELING

Egorov B.V.[1], Koshcheev A.V.[1], Markachev Yu.E.[1], Plekhanov E.A.[1], Tchougreeff A.L.[2], Ufimtsev I.S.[1]
[1]- Central Aerohydrodynamic Institute,
[2]- Institute of Physical Chemistry,
bv-egorov@yandex.ru, tch@hcc.keldysh.ru

Formation of the simplest neutral and charged clusters $(H_2O)_n$, C_n, $SO_2(H_2O)_n$, $SO_3(H_2O)_n$, $H_2SO_4(H_2O)_n$, $H^+(H_2O)_n$, $OH^-(H_2O)_n$ etc. in conditions of an active aircraft discharge compensator and exhaust jet is studied in this work. The calculations of the structure and energetics of these clusters are carried out by means of *ab initio* quantum chemistry methods. The data of quantum chemical calculations are used to obtain the dissociation energy and partition functions of different kinds of internal movements for all clusters considered to calculate equilibrium constants for kinetics with single monomer association and dissociation. Dissociation rate constants are estimated by monomolecular decay theory and formation rate constants are calculated using equilibrium constants.

Within the framework of created neutral and charged cluster kinetics it was carried out numerical modeling of: 1) the flow in the tract of active compensator of electricity of an airplane; 2) the flow in engine exhaust jet behind the perspective supersonic passenger aircraft; 3) the flow in nozzle and working section of some TsAGI wind tunnels.

It was shown that $H^+(H_2O)_5$ clusters are responsible for the main fraction of corona discharge current in aircraft active compensator in conditions of wet low troposphere (water vapor mole fraction of 3%). The basic carriers of electrical charges in discharge channel in conditions of dry air of low troposphere (water vapor mole fraction of 10^{-6}) are hydrates of oxygen negative ions.

Numerical densities of neutral clusters and sulfur acid molecules along exhaust jet behind prospective second-generation supersonic

transport aircraft in stratospheric flight at 18 km altitude were calculated based on traditional chemistry as well as cluster chemistry considered. It was shown that in initial stage of sulfur acid aerosol generation the basic channel is the channel with participation of sulfur trioxide and water vapor dimmers.

It was shown that formation of neutral and charged clusters of working gas in aerodynamic facilities at certain modes of operation influences essentially on optical, gasdynamic, thermal and aerodynamic characteristics of flow simulated.

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LACK OF SCIENTIFIC CONTENT IN NONEQUILIBRIUM STATISTICAL PHYSICS

Erofeev V.I.
Institute of Automation Electrometry, yerofeyev@iae.nsk.su

Consideration of nonresonant electron diffusion in an idealcollisionless plasma with Langmuir turbulence revealed an irrationality of ensemble method[1]. After Tsytovich [2], it was commonly believed that this diffusion never leads to decay of Langmuir quanta. But traditional theory recognizes as well results that comprise intense wave quanta decay (see details in [1]). It arrests wave spectral transfer (and henceprecludes formation of Langmuir wave condensate)[1], suppresses Vedenov-Rudakov's plasma modulational instability, and prevents Zakharov's Langmuir wave collapse[3].

That is, it violates drastically all basic conceptions of traditional plasma turbulence theory. The difference of two pictures of electron diffusion originates from traditional substitution of real plasma by plasma probabilistic ensemble. Their authors implied ensembles with different properties, and substantial suppression of the process intensity in one of them as compared to another shows that generally the ensemble averaging obscures real picture of physical phenomenon to an indefinite degree. Noteworthy that idea of intense wave quanta decay complies with absence of Langmuir wave collapses in two independent series of beam-plasma experiments with strong Langmuirturbulence (see analyses of experiments in [1,3]).Consideration of nonresonant electron diffusion with refraining from ensemble substitution also confirms idea of intense decay of Langmuir quanta [1,3].

Conclusion about absence of any sense in studies of evolving plasma ensembles is confirmed also by Langmuir wave scattering induced by plasma electrons. New calculations show that waves with wavelengths $r_D \le \lambda < m?M^{2/5} r_D$ scatter with essentially higher intensity than it was formerly deduced~[4]. Their Compton scatterings on a single electron competes successfully with scatterings on its ``shielding cloud", and details of electron distribution in real plasma become important. Being ensemble-averaged, bulk of the corresponding coherent wave scatter was smeared out.

Thus, the ensemble studies cannot help one to develop objective picture of the system physical evolution. With this, conceptions of sciences based on ensemble method up to statistical physics in general need a thorough revision.

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THE KINETIC FOUNDATIONS OF GENERALIZED NON-EQUILIBRIUM THERMODYNAMICS OF MULTICOMPONENT GAS MIXTURE

Zhdanov V. M.
Moscow Engineering Physics Institute, svetlova@istc.ru.

The problems of the kinetic foundations of the generalized nonequilibrium thermodynamics of multicomponent gas mixture based on the linearized equations of Grad's moment method are discussed.

The infinite hierarchy of the coupling equations for the expansion coefficients or the set of the moment equations is derived on the base of the linearized Boltzmann kinetic equation. The generalized expressions for the local entropy density, entropy flux density and local entropy production are obtained on the kinetic level. The alternative versions of the linear relations between the fluxes and the generalized thermodynamic forces are discussed. For the homogeneous state of the system the relations are in agreement with the Onsager version of the linear irreversible thermodynamics. In the case of the non-homogeneous systems the expressions for the thermodynamic forces are complicated and include the time and the spatial derivatives of the fluxes (moments) along with the usual gradients of the standard thermodynamics variables. The results for the simple (one-component) gas are in good agreement with those obtained by the methods of so-called extended irreversible thermodynamics. Some consequences and new physical phenomena followed from the results obtained are discussed. An application of perturbation theory in the small Knudsen number to the system of moment equation yields results that are identical to the results of the Chapman- Enskog method at the level of both the first and second (Burnett) approximation.

THE LINEARIZED MOMENT METHOD IN THE KINETIC THEORY OF MULTICOMPONENT GAS MIXTURE. HIGH APPROXIMATION

Zhdanov V. M., Roldugin V.I.
Moscow Engineering Physics Institute, svetlova@istc.ru.

The method of the moment equations derivation on the base of linearized Boltzmann kinetic equation is developed when the expansion of the distribution function in series over irreducible tensorial Hermite polynomials is used.

It is shown that the terms with the spatial derivatives of the fluxes (moments)in the moment equations should be taken into account. Without these terms and after a time interval equal to some mean times between the collisions of the particles the moment equations reduce to the algebraical system of the equations for the expansion coefficients in any order of approximation. The expressions for the heat flux in the multicomponent gas mixture and the equations for the diffusion fluxes written in an easy-to-use Stefan- Maxwell form with the consideration for multicomponent thermal diffusion are derived. It was shown that the kinetic coefficients of the multicomponent gas mixture can be written s the ratio of two determinants of the lowest order than the similar expression which obtained by the standard Chapman-Enskog method. The calculation of the kinetic coefficients in any approximation over the number of Sonine polynomials in the expansion is noticeably simplified.

RESEARCH OF THE CHEMICAL REACTIONS INITIATED BY AN ELECTRON BEAM IN A FLOWS OF A PURE METHANE AND ITS MIXES

Zarvin A.E., Madirbaev V.Zh., Sharafutdinov R.G.
Novosibirsk State University. zarvin@phys.nsu.ru

By means of molecular beam mass-spectrometry the researches of the composition of a flows of pure methane and its mixes activated by an electron beam are executed. The work was carried out on a pulse gas-dynamic installation LEMPUS of Novosibirsk State University and a vacuum setup VS-4 of Institute of Thermophysics of SB RAS. The opportunity of input of activated electron beam as across, as along an axis of a gas flow was supplied. The vacuum setup VS-4 is equipped also by the flowing quartz reactor.

It is shown, that the molecular beam mass-spectrometric systems provide the registration of changes of a neutral component in a gas flow at initiation of plasmachemical reactions in both variants of accommodation of an electron guns. The problems arising at joint sharing of an electron beam and the mass-spectrometric equipment are considered.

It is revealed, that at activation of gas by an electrons the fall of concentration of methane and occurrence of molecular hydrogen in a flow is observed. Shown, that this effect is caused by the fast ion - molecular reactions proceeding in the reactor. The dependence of fac-

tor of conversion of methane to hydrogen from the concentration of methane, current and energy of activated electrons is measured.

At expansion of gas to the vacuum the condensation is observed. The presence of clusters, is especial in plasma, essentially influences on gas-phase processes. We investigated the influence of condensation in a flow on the conversion of methane to hydrogen. For this purpose are executed the mass-spectrometric measurements of the composition of molecular beam generated from supersonic free jets of gas mixes $50\%CO_2+50\%CH_4$, $Ar+5\%CH_4$, $Ar+5\%CO_2$ in a wide range of parameters of the expiration, in that number in conditions of intensive condensation. The measurements of intensity of monomers and small clusters were made depending on stagnation pressure P_0.

The opportunities of use of the received results for development of a technique of plasmachemical processing of a mix of methane and carbon dioxide to the synthesis gas are considered.

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ACTUAL RAREFIED GAS DYNAMICS PROBLEMS IN SPACECRAFT DESIGN AND MAINTENANCE

Zvorikin L.L., Krylov A.N., Mishina L.V.
RSC "Energia", Andrey.N.Krylov@rsce.ru

Actual rarefied gas dynamics problems arising from spacecraft design and operation, space scientific and technological investigations are under discussion in the report.

For a long time RSCE specialists successfully applied rarefied gas dynamics methods to spacecraft design and operation problems beginning nose fairing jettisoning at injection stage, including orbital flight until descent stage. Modern hardware and software give possibility to solve such problems for altitude higher then 80 km. Some examples of solved aerodynamics problems in free molecular and transient flow regimes are given.

The actual problems of own spacecraft ambient atmosphere parameters assessment, its dynamics under orbital flight conditions and an effect on spacecraft devices and systems are also under consideration. The solving of these issues is necessary for reliable operation of spacecraft systems, for correct definition and realization of technological and scientific experiments which pose high requirements to ambient atmosphere clearness and vacuum level stability. The numerical investigation results of screening effect of cross-flowed disk under orbital conditions are presented. It is shown the possibility of high vacuum stable zone occurrence with rarefaction levels irreproducible in earth-based conditions.

The problems of mass transfer in peripheral part of underexpanded thruster plumes and their force and thermal action on spacecraft elements are discussed. It is shown that complex configuration of modern high orbital satellites leads to the necessity of solving the problem of an interaction of two and more underexpanded plumes with each other and spacecraft structure. Widespread cold gas thrusters need to take into account the condensation effects within gas flux and to pay particular attention to gas - surface interaction. The analysis is made concerning the possibility of rarefied gas dynamics method applicability to fluid exhausted into the vacuum problem being an important one for orbital station operation.

The review of on-board space experiments in rarefied gas dynamics fields made by RSCE is done and directions of future investigation are determined.

SURFACE SCREENING BY THIN DUSTY LAYER OF CHARGED METAL CLUSTER

Zmievskaya G.I. [1], **Levchenko V.D.** [1], **Levchenko T.V.** [2], **Soboleva T.K.** [3]

[1] - Keldysh Institute of Applied Mathematics of RAS
[2] - VNITs GEOINFORM, Research Center,
[3]- Instituto de Ciencias Nucleares,
Universidad Nacional Autonoma de Mexico,
zmi@keldysh.ru

Charged condenced metal liquid droplets or disperced powders in the technological devices can appear due to surface erosion. Both droplet and dust cloud change electrode screening processes and decrease energetic plasma flow towards the surface. Screening conditions depend on metal droplet sizes due to vapore condensation, cluster concentration in the near vicinity of electrode as well dust particles charging.

Dusty plasma kinetic 3D3V code SUR Dust [1] put forward. As a first step to estimation of plasma heat and particle flow attenuation we use 1D hydrodynamical code [2], based on plasma model [3]. In contrast to [2,3] constant cross-sections plasma-dust particles interaction were replaced by effective cross-section of ions and electrons scattering, received from high explicit computer simulation 3D3V code [1].

The distribution of metal droplet versus its sizes in dusty layer can be simulated by stochastic analog method [4] under conditions similar to plasma model [2]. The varied parameters of dusty layer model are follows: charged droplets concentration, radius and charge of clusters and so on. Screening effect is investigated by computer simulation .

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DIRECT STATISTICAL SIMULATION OF REAL GAS EFFECTS

Ivanov M.S., Gimelshein S.F., Bondar E.A.
Institute of Theoretical and Applied Mechanics, ivanov@itam.nsc.ru

Wide application of the method of direct statistical simulation (DSS) for solving the problems of rarefied gas dynamics stimulated the last decade intensive development of models for the accounting of real gas effects. From the point of view of the kinetic theory the concept " effects of real gas " includes various phenomena connected with collision processes, such as energy exchange between translational and internal modes of molecules, chemical reactions, ionization and radiation. The method DSS requires physically proved models describing various types of the intermolecular interactions exactly enough. These models should also possess a high numerical efficiency; that is especially important for the flows simulation at low Knudsen numbers. Last years a number of exact models based on the application of the results of the quasi-classical and quantum theories were offered. However the lack of experimental data makes it impossible to use these models for many important problems in which it is necessary to consider polyatomic molecules. The purpose of the present review is the discussion of modern models of the method DSS for the description of the real gas effects.

The following points are discussed in detail.

- *The models for the accounting of the translational-rotational and translational-vibrational energy exchange.* The main attention is paid to the most general model of the existing models – Larsen -

Bornakke model, which is the only one really applicable to polyatomic molecules today.

- *The description models of chemical reactions.* The widely used total collision energy model (TCE, Bird 1978), and the model with preference of vibrations and dissociations are both discussed.
- *Methodology of a choice.* The algorithm of simulation of inelastic collisions in the DSS method is submitted. It allows achieving of the exact performance of Jeans and Landau-Taylor relations for the relaxation rate of the rotary and vibrational energies.
- *The continual and the discrete description of the internal energy of molecules.* The key differences of these two approaches used in the DSS method are discussed. The advantage of the use of the molecular vibrational energy discrete description is shown.
- *The rates of chemical reactions for the discrete approach.* The algorithm of correcting of the reaction rate constants in the Arrhenius equation is submitted. The algorithm allows achieving the agreement of the reaction rate with its theoretical value for the equilibrium case.

3D3V KINETIC MODELING OF INTERACTION OF PLASMA FLOW WITH DUST PARTICLES.

Inkov L.V., Levchenko V.D. Zmievskaya G.I.
Institute of Applied Mathematics

During the last decade, an extremely rapid growth of dusty plasma physics take place. It can be accounted for the laboratory experiments in which a number of interesting phenomena were discovered and for the important technological applications in plasma etching and deposition [1].

Most processes in dusty plasma are by definition non-equilibrium and non-stationary. That's why the kinetic approach in numerical simulation of dusty plasma is advisable [2].

Full kinetic self-consistent 3D3V numerical model of dusty plasma has been built. It takes into account strong collisions of particles with dust grains. The model is implemented in a framework of universal kinetic PIC 3D code SUR [3].

Test computations of the modeling problems verified the effectiveness of the code. The dependence of results from modeling parameters was examined. The restrictions on modeling parameters were determined.

The problem of scattering of the plasma flow on a dusty cloud near the wall was solved. The dependence of cross-section of flow loss from dust density and grain radius was examined. It was shown, that the distribution function of the flow become strongly non-equilibrium due to the interaction with the cloud [4].

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APPLICATION OF COMBINED SPHERICALLY SYMMETRICAL POTENTIAL OF INTERMOLECULAR INTERACTION FOR CALCULATION OF ISOCHORIC HEAT CAPACITY OF RAREFIED GAS.

Kaplun A.B. [1], **Meshalkin A.B.** [1], **Abdulagatov A.I.** [2], **Abdulagatov I.M.** [3], **Stepanov G.V.** [3]
[1]- Institute of Thermophysics, kaplun@itp.nsc.ru
[2]- Institute for Geothermal Problems of RAS, Makhachkala, magur@datacom.ru
[3]- Institute of Physics of the Dagestan Scientific Center RAS.

At present time it is possible to calculate virial coefficients ($B(T)$, $C(T)$, and etc.) and their temperature derivatives with used of model

potentials of the intermolecular interaction what is allows to calculated of some properties of rarefied gas - heat capacity for example. Earlier we proposed the combined spherically symmetrical potential of intermolecular interaction [1] for calculation of second virial coefficient of the nonpolar substances in all experimental investigated temperature range within their experimental uncertainties including helium and hydrogen having an essential quantum component. This potential of intermolecular interaction was modernized taking into account Keesom' forces for dipole - dipole interaction and can be applied for description of the polar molecules interaction such as water, ammonia and alcohol's.

In paper are reported about carry out measurements of isochoric heart capacity of argon, carbon dioxide, water, n-pentane, n-octane and 1-propanol in the wide temperature range by the method described in [2]. For this substances values of first and second temperature derivatives of the second virial coefficient $2 \cdot T(dB/dT) + T^2(d^2B/dT^2)$ on base of data are obtained in experiments and are make a comparison with recommended values of virial equations of state and experimental values of the isobaric heat capacity. It is shown that the proposed combined spherically symmetrical potential of intermolecular interaction is allowed to describe experimental data within their experimental uncertainties in general, and it can be useful for interpolation and extrapolation of the experimental data.

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PHOTOPHORETIC FORCE MEASUREMENT BY KNUDSEN NUMBER SIMULATION TECHNIQUE

Kovalev F.D., Shishkin A.D..
Ural State University, Ekatherinburg

Different experimental methods for photophoresis phenomenon investigation analized. Their advantages and possibility of atmospheric aerosol dynamics simulation evaluated. Magnitude and typical values of main parameters of aerosol particles and gases were evaluated. Performance evaluation of a Knudsen number simulation technique for photophoresis investigation was demonstrated. For number of selected model particles optical and thermal properties was measured. Photophoretic force measured with torsion balance with electrostatic compensation by null reading method for selected particles in helium, argon and air at light intensities 800 - 3000 W/m^2 in wide range of Knudsen numbers (0.01 - 10). Most attention has been concentrated on minimization of experimental errors to provide a possibility of accurate comparison our experimental results with theoretical prediction. Specifically, the light intensity measurement tract and original method of particle optical parameters evaluation developed. The temperature distribution on particle surface investigated for limit cases of positive and negative photophoresis.

For bulk graphite, steel, glass particles a good agreement of experimental results and theory was observed. In case of polystirol particles at large Knudsen numbers and increasing of light intensity some systematic deviations from theoretic prediction observed.

PHOTOPHORESIS STUDY USING VIDEO DATA METHOD

Kovalev F.D., Shishkin A.D..
Ural State University, Ekatherinburg

The intention in present study is to evaluate capabilities of video-data technique for phoretic phenomena with aerosol particles suspended in gas. Photo-, thermo- and dif-fusioforesis consist in force occurrence acting a particle and due to non equilibriumstate in gas-particle surface system. The video-data method consists in recording ofaerosol particle motion by a VHS-recorder and computer processing of video-image.The method provides opportunities to

determine particle coordinates as a function oftime, any changes in its motion under various experimental conditions. It is also possible to obtain particle size and density. The video-data technique was applied in experiment on photophoresis. Particle steady-state velocity in this case results from gravity, photophoretic and convective drag forces. One of the first quantitative examination of photophoresis provided by Rosen M.N. and Orr C. in 1963 was based on observation of aerosol particles drift. Present experimental idea is similar. An additionalpoint to emphasize is that photopheresis is good enough investigated so experimentalresults could be correctly compared with exist theoretical models.The results in free molecular regime is in good agreement with theory. At Knudsennumber smaller than unit the convective drag force is to be taken into account.It is possible to conclude that television method of particle movement observation issuitable for photophoresis investigation and may be used for experiments onthermophoresis and diffiisiofbresis

STATISTICAL EQUILIBRIUM ACCORDING TO GIBBS AND POINCARE

Kozlov V.V.
Mathematical Institute of RAS, kozlov@pran.ru

According to Gibbs, the density of probability measure as a function of canonical coordinates and time satisfies the Liouville equation. The stationary densities of distribution correspond to the statistical (thermal) equilibrium of the dynamic system. Gibbs tried to show, that the Hamilton dynamic system approaches an equilibrium state (in a sense) at an unlimited increase of time. However (according to the Poincare return theorem) the density of probability measure has no limit in usual sense at all. It is useful to replace the usual convergence with the weak convergence, as we are interested only in the behavior of the average means of dynamic values at the transition to the macrodescription.

In the report it will be told about new results in the problem of weak convergence of the Liouville equation solution for nonlinear Hamilton systems and about their application to the kinetics of the continuous medium without collisions. It sheds new light on the old problem of irreversibility. In particular, the Gibbs entropy as a function of time is constant, however at $t \to \pm\infty$ it has the same non-negative jump which magnitude quite agrees with the data of thermodynamics.

The results of the general theory will be illustrated with an effective example of the kinetics of the continuous medium without collisions in a box with perfectly reflecting walls. For the first time this theory was considered by Poincare in the work of 1906 (unfortunately, not understood). It appears, that such gas tends irreversibly to fill this box homogeneously, irrespective of the initial distribution. Thus the equations of motion of the medium without collisions are invariant at the time reversal, and each particle approaches the initial position infinitely close. The mechanism of irreversibility is caused by non-uniformity of the time of returning.

ON THE LOGICAL STRUCTURE OF RAREFIED GAS DYNAMICS

Kolesnichenko E.G., Vartazarian T.A., Ivanov D.I.
Institute of Mechanics, MGU, egkol@yandex.ru

The creation of information systems for the different areas of knowledge demands to work out the logical structure of these areas. In this report we discuss one of the possible approach to the logical organization of rarefied gas dynamics. We consider this science as a rather complicated collection of mathematical models. Each mathematical model can be represented by some set of formal theories in the first order predicate logic. The solution of the problems stated became essentially simplified when we have some unified description of all mathematical models. As a such one we propose the algebraic axiomatization of quantum mechanics in which the model is represented as a union of : 1) algebra of observables, 2)the space of states, 3) the semigroup of endomorfisms which determines the evolution of model in space and time. The notion of scientific knowledge contains also the methatheoretic information about the relations between different models and their attributes. For the description of such methatheory it is necessary to formulate the corresponding language, that is to determine these attributes and relations. They can be divided on the groups according their pragmatic functions. The possible choice of such func-

tions is discussed. In particular in the rarefied gas dynamics the relations of asymptotic deductibility of one model from another are important. The problems, connected with these relations are discussed as well as the problem statements determined by the general goal of the creation of information system. In the frame of our project it is supposed that the logical structure can be described with help of XML and Xlink and Xpointer languages. This impose some restriction on the representation of information which are discussed in the report/ We believe that the creation of the information systems of the tipe described is possible only with the participation of all scientific community. Then some organization problems arises. As a one of the possible ways of the solution of this problems we have organized the electronic journal "Physical chemical gas kinetics in the gas dynamics." On the sites www.chemphys.edu.ru and www.csa./Avogadro .

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MODELING OF SUPERSONIC UNDEREXPANDED FREE JETS BY THE EXPANSION FROM A PULSE SOURCE

Korobeyshchikov N.G., Zarvin A.E., Madirbaev V.Zh., Sharafutdinov R.G.
Novosibirsk State University. zarvin@phys.nsu.ru

The purpose of the present work is the research of a correctness of modeling of a stationary processes in supersonic jets of low density by the pulse expansion. The experiments are executed on a complex of gas-dynamic installations LEMPUS of Novosibirsk State University and on the vacuum setup VS-4 of Institute of Thermophysics SB RAS by methods of an electron-beam spectroscopy and a molecular-beam mass-spectrometry. The outflowing into the evacuated space of the pulse underexpanded jets of the helium, argon and nitrogen with moderate and large degrees of underexpanding is investigated. The degree of underexpanding varied in the limits – 10^3 - 10^6.

Is shown, that on the fixed distances from a source the experimental measurements of the time of an establishment of a parameters appropriate to the stationary flow for different modes are generalized

in the dimensionless coordinates and will be coordinated to the theory [1].

The limits of the area of a quasi-stationary flow on the different distances from a source are determined. Is shown, that the duration of quasi-stationary area decreases at movement of a gas pulse downwards on a flow, and also at increase of a pressure of background gas.

It is established, that the experimental results of measurements of the intensities of a gas pulses in a wide interval of the stagnation pressure P_0 and the distances from nozzle x/d* are generalized at use of a parameter of similarity Re_L.

The direct experimental check of the equivalence of pulse and continuous free jets is carried out. For this purpose the comparison of the data on longitudinal structures of density measured with the help of an electron beam diagnostics in a supersonic jets of nitrogen and argon, on abnormal fluorescence of atomic argon in a mix of argon and monosilane, activated by an electrons, and also the results of a study of condensation in jets of argon, executed by the methods of the molecular-beam mass-spectrometry is carried out.

The conditions are found, at which the results of a pulse and continuous measurements are equivalent. The borders of applicability of the pulse expansion for the modeling of continuous flows are determined.

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PHOTOPHORESIS OF AEROSOLS IN THE UPPER EARTH'S ATMOSPHERE

Kochneva L.B., Beresnev S.A, Suetin P.E.
Ural State University, Ekaterinburg, Sergey.Beresnev@usu.ru

The opportunity of a levitation (and even of vertical lifting) particles of particular types of atmospheric aerosol on high altitudes under the action of photophoretic forces is considered some decades. The numerous observation facts testify to presence and anomalously continuous stay in the stratosphere of carbon particles of the different nature, volcanic aerosol etc. The major concern calls a problem on the nature and formation conditions of stable aerosol layers at different heights in stratosphere and mesosphere, most known from which one are the Jounge layer, polar stratosphere clouds and polar mesospheric (noctilucent) clouds. All these facts give reasons for searching and analysis of microphysical force mechanisms exhibited in particular requirements of high altitudes and providing vertical transport of aerosols against gravity. The traditional models of vertical aerosol transport based on idea of sedimentation-diffusion equilibrium are not capable to describe apparent aerosol stratification at different altitudes in stratosphere.

By the possible and justified reason of motion of atmospheric aerosol particles against gravity the contributors consider the radiometric photophoresis. The correct estimations of "power opportunities" of photophoresis are farly from being finished. The reason it is the complexity of this phenomenon and necessity both the electrodynamic and the gas-kinetic case study. In this report the results of gas-kinetic theory of photophoresis for description of vertical transport of atmospheric aerosols are presented. Three basic models are considered: 1) conventional negative photophoresis of aerosols in a solar radiation field, 2) photophoresis of aerosols in the thermal (infrared) Earth' radiation field, 3) combined model. The estimations from the first model show that the negative radiometric photophoresis is capable to cause a levitation black carbon particles of different types of a some size range and thermal properties at different altitudes in the stratosphere. The estimations on second, original and not explored before model, also give in deductions about levitation opportunity and vertical lifting of particles of a some types of atmospheric aerosols. The perspectives of usage of the obtained results for development of new model of vertical transport of stratospheric and mesospheric aerosols are considered, where alongside with conventional mechanisms

(gravitational sedimentation, the Brownian diffusion etc.) is taken into account also the photo- and thermophoretic particle motion.

GAS-DUST MIXTURE FLOW AT THE PRESENCE OF EVAPORATION-CONDENSATION ON SOLID PARTICLES

Kryukov A.P., Levashov V.Yu., Shishkova I.N.
Moscow Power Engineering Institute, KryukovAP@mpei.ru

The problems of strong non-equilibrium vapor-gas mixtures flows through the domain filled by solid particles are studied in this paper. Presented analysis takes into account dust particles sizes variation owing to the evaporation-condensation processes on the dust surfaces. The velocity distribution function of gas molecules is found from the direct numerical solution of the Boltzmann kinetic equation [1]. The approach for calculation of the distribution function transformation as result of gas molecules and dust particles interactions is used [2]. In [3] the problem of gas flow through the region occupied by solid particles at the presence of condensation has been investigated, however at this particles sizes were considered as constant values.

Evaporation-condensation problem in the volume filled by dust particles is considered. At this the following suggestions are made and conditions are formulated. At the initial time moment ($t=0$) spherical solid particles are distributed in the domain uniformly with numerical density $4.83*10^{20}m^{-3}$. The diameter of these particles is $93.8*10^{-10}m$.. It is assumed that gas (nitrogen) temperature at the entry in flow region is T_0=300K and pressure P_0 = 20kPa, temperature of particles surfaces is suggested to be constant and equal to 300K. Particles sizes variation depend on quantity of gas molecules deposited on the dust at the prescribed value of condensation coefficient, and quantity of gas molecules emitted from the dust during evaporation also. Quantity of gas molecules, which hit the dust is determined for each cell of investigated domain in the solution process. It is assumed that evaporation is realized on the dust particle surfaces in accordance with diffuse scheme. Thus it is considered that vapor molecules emitted from the dust surface have Maxwell distribution function with temperature of

this surface, known saturation density corresponding to this temperature and zero flow velocity.

The distributions of gas macro-parameters and solid particles diameters in the flow region are presented for different time moments, values of condensation coefficient and vapor saturation density.

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STUDY OF NON-STEADY HEAT TRANSFER IN VAPOR FILM BY NUMERICAL SOLVING OF THE BOLTZMANN EQUATION

Kryukov A.P., Yastrebov A.K.
Moscow Power Engineering Institute, apk@mcsa.ac.ru

Solution of the Boltzmann kinetic equation for non-steady heat transfer in vapor film was obtained. Conservative discrete ordinates method [1] was used. The applied splitting procedure is that at any time step the equation of free-molecular flow is solved firstly and then the equation of uniform relaxation is solved. The second-order

SHASTA algorithm [2] was used for equation of free-molecular flow solving. Its main advantage is that used coordinate step can be more than mean free path, so calculation time can be decreased.

Boundaries of considered vapor film were two flat and parallel surfaces, one of them is non-penetrable for mass flux (heater), other surface is penetrable (interphase surface). Problem was considered as one-dimensional. Before beginning of process the whole system is in equilibrium state at temperature of interphase surface, heat flux is zero. At initial moment of time heater temperature increases or heat flux on the heater increases. Because vapor temperature near the heater increases, pressure becomes greater than saturation pressure at interphase surface temperature, so vapor is condensed during the non-steady process. It is obvious that mass flux does not depend on coordinate in steady state. Mass flux on heater surface is always zero, so mass flux in steady state is also equal to zero. This qualitative description is in agreement with carried out calculations. If film thickness is relatively small (Knudsen number is more than 0.005) duration of non-steady process is very small. For example, if considered substance is helium, interphase surface temperature is 2 K, and Knudsen number is 0.005 (corresponding to film thickness 6 micron) non-steady process lasts about 1 microsecond.

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INFLUENCING OF TRANSLATIONAL NONEQUILIBRIUM ON RATE CONSTANTS OF CHEMICAL REACTION IN SHOCK WAVE IN HIGH-ENTHALPY GAS FLOW

Kuznetsov M.M., Komarov V.N., Yumashev V.L.
Central Aerohydrodynamic Institute, Yumashev@falt.deep.ru

On the basis of molecular-kinetic model "beam - continuum" [1] the structure of the shock wave in the chemically reacting gas flow with the high enthalpy containing a noticeable part of the dissociation energy of molecules is reviewed. The calculations have shown, that the high enthalpy of the flow can result in to essential reduction of the energy barrier of such reactions, that results in considerable increase of the conforming rate constants. For the first time strong dependence of the rate constant of translational-nonequilibrium bimolecular chemical reaction from macrovelocity of flow was established in paper [2]. In the present paper the rate constant of translational-nonequilibrium chemical reaction is determined for the case of arbitrary relation of cross-section of collision from energy of relative movement of molecules. Some outcomes of calculations of translational and chemically nonequilibrium air in a shock wave are given.

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TRANSPORT PROCESSES IN STRONGLY NONEQUILIBRIUM GASES. KINETIC THEORY AND APPLICATIONS

Kustova E.V., Nagnibeda E.A.
Saint-Petersburg State University, vnag@vnag.usr.pu.ru

Under the conditions of strong deviations from the equilibrium the characteristic times of vibrational and chemical kinetics in a gas flow are comparabale with the mean time of gas dynamic parameters changing. Therefore gas dynamic equations should be considered together with the equations for vibrational level populations and atomic number densities. Nonequilibruium distributions can influence significantly on gas dynamics and transport properties in the flow.

The present paper deals with the modelling of transport properties in reacting gas flows taking into account strongly nonequlibrium vibrational distributions. The paper presents the main principles of the transport kinetic theory in gas flows under the conditions of strong vibrational and chemical nonequilibrium [1]. The applications of this theory to the flows of reacting mixtures behind shock waves, near the surface of re-entering body, in nozzles [2,3,4] are discussed as well.

The comparison of the results obtained using state-to-state distributions and ones based on multi-temperature and one-temperature quasi-stationary distributions is shown and the limits of the validity commonly used multi-temperature models are discussed.

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NUMERICAL METHOD FOR SOLVING BOLTZMANN'S EQUATION AT LOW KNUDSEN NUMBERS

Larina I. N, Rykov V. A.
Computing Center RAS, larina@ccas.ru

Computation of rarefied gas flows at low Knudsen numbers is impeded by certain difficulties. They are explained by the fact that numerical viscosity tends to suppress the effects due to physical viscosity and heat conduction as the Knudsen number is decreased while the grid in the physical space is held invariant. These difficulties are primarily characteristic of first-order accurate schemes. To reduce numerical viscosity, the mesh size in space must be smaller than the Knudsen number, which leads to an unwarranted increase in the number of cells in the physical space. In this paper, we propose a numerical scheme that is second-order accurate in time and space for solving Boltzmann's equation at low Knudsen numbers. The method is based on the well-known idea of splitting the gas motion into the sequence of relaxation and free-molecular stages [1-2]. Since the gas motion is analyzed at low Knudsen numbers, the distribution function is close to a locally Maxwellian one and can be represented as the sum of a locally Maxwellian distribution function and a small nonequilibrium term. In terms of time complexity, the computational cost of the method is primarily due to the gas-relaxation stage. An efficient solution of the relaxation problem is based on a linearization of the collision integral about the locally Maxwellian distribution. The locally Maxwellian distribution function is represented in a canonical form that does not involve any explicit dependence on macroscopic flow characteristics. This is done by changing from the absolute particle velocities to thermal velocities divided by the square root of temperature and normalizing the function to unit density. A discrete representation of the collision integral is obtained as the product of a constant collision matrix and components of the vector of cell occupation numbers. A preliminary calculation and storage of the matrix make it possible to speed up computation of the gas-relaxation stage. The free-molecular stage is computed so that the number of particles, momentum, and energy are conserved. The method is used to compute the structure of a

shock wave and a problem in heat transfer. The resulting solutions are compared with the well-known solution to Boltzmann's equation .

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ANALITIC SOLUTION OF THE SECOND ORDER THERMAL SLIDE PROBLEM

Latyshev A.V., Popov V.N., Yushkanov A.A.
Pomor State University, Arkhangelsk, popov.vasily@pomorsu.ru

The problem of a second order thermal slide velocity of a rarified gas over a solid surface is solved by the using of three models of the Boltzmann kinetic equations (BGK model with a constant collision frequency, ES-model and BGK model with a collision frequency proportional to the absolute quantity of a molecular velocity). In all cases the general solution of model kinetic equations are constructed in the generalized functions space. By substitution in the obtained general solutions original boundary conditions the singular equations with the kernel in the Cauchy's form are obtained. By using Sohotsky-Plemel's formulas the obtained singular equations are reduced to the Riemann's boundary problems. The founded second order thermal slide velocity is obtained from the solvability conditions of the constructed boundary problems. The follow meanings of the coefficient taking into account the influence of the curved of the surface on the slide velocity for the three using models of the Boltzmann equations are obtained: 2.376842, 1.834375 и 1.1437.

The results those are obtained by the using the BGK model with a constant collision frequency and the ES-model confirm the existence

of the negative (in the direction of the gradient of a temperature) thermophoresis of a high thermal conductive aerosol particulars at small meanings of the Knudsen numbers.

The results those are obtained in this paper let us to make a conclusion about an essentially dependence of the meaning of the second order thermal slide coefficient from the choice of the model of the collision integral.

CLUSTER-IONIC INTERACTION IN SUPERSONIC JETS OF GAS MIXES AT ELECTRON BEAM OF ACTIVATION

Madirbaev V.Zh., Zarvin A.E., Sharafutdinov R.G.
Novosibirsk State University, madirbaev@phys.nsu.ru

In 1999 it was revealed, that in supersonic jet of a mix of argon with monosilane, activated by an electron beam, the diagram of dependence of radiation intensity of separate lines of atomic argon from the stagnation pressure P_0 at some meanings of P_0 begins to grow nonlinearly [1]. A range of display of this effect and its reasons became a theme of the present work. The researches carry out on the installation LEMPUS [2]. In work were used pure argon and its mix with methane, monosilane, carbon dioxide and helium. The dependences on pressure of intensities of radiation of separate lines of atomic (λ = 549,6 nm) and ionized (λ = 450,9 nm) argon and impurity were registered. These data were compared to the results of mass-spectrometric measurements of composition of molecular beam generated from the researched jet.

It was revealed, that the beginning of abnormal effect corresponds to the beginning of condensation in a flow, its ending corresponds to complete transition of molecules of an impurity to the clusters, intensity of an optical signal linearly depends on a current of an electron beam, and the lifetime of excitation is much greater of optical lifetime of excited states of argon.

The specified features have allowed to make the assumption, that the effect arises owing to ion-cluster interaction initiated by an electron beam plasma. In a flow are formed the long-lived exited complexes including as atoms of the gas - carrier, as the particles of an impurity. After transfer of excitation to the radiating states of atomic argon occurs, apparently, ejection of argon from the cluster and the subsequent emanation of photon. The model of the process of cascade selective excitation of atomic argon in a mix is constructed, its experimental verification is executed.

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FLOWS IN THE NARROW CHANNELS: ANALYTICAL AND NUMERICAL SOLUTION

Memnonov V.P.
S.Petersburg State University, pokusa@star.math.spbu.ru

Current trend toward nanotechnology often causes some of linear dimensions of contemporary high-tec devices to be of order of a molecular mean free path λ already under the atmospheric pressure. Thus these flows are in transitional regime and direct simulation Monte Carlo (DSMC) method is quite suitable for their numerical modeling.

Two problems of the Monte-Carlo simulations in narrow channels are considered. First we present the results of simulations by the DSMC method for two-dimensional unsteady problem of gas flow in a narrow channel with an inclined upper wall and a moving lower one. This is a model of gas film lubrication in modern magnetic disk

storage, which are now being under development. Due attention is given to non-uniform inner and external structure of the boundary incoming and outgoing flows. This is carried out by simultaneous continuum finite element solution for the external flow over the magnetic head and using its results as boundary conditions for DSMC simulations. Pressure, density and velocity distributions along the channel as well as before its inlet were obtained. Unlike the assumptions in the previous papers on the topic the latter are shown to be badly non-uniform.

In the other problem of the DSMC simulation for filter flow with extremely small mean gas velocity the most serious difficulty was large statistical scattering, which has been surmounted by enlarging the samples through Internet connection of several clusters into a metacomputer. Special dynamic load balance technique under our distributed memory conditions was developed. The quantitative estimation of its performance has shown that efficiency of using processors inside our metacomputer was only 2% - 3% lower than for computation on the same cluster without Internet connection. Numerical simulation results for filter problem also are given.

Yet in some cases it is important to study very long channels up to 20000 λ. But this is far beyond the present computing capabilities. For these cases it is suggested to couple the DSMC simulation at the entrance and exit of the channel with an asymptotic solution of the Boltzmann's equation in between.

THE SIMPLE EQUATION FOR CALCULATION OF THE VISCOSITY LIQUID AND GAS OF NORMAL SUBSTANCES

Meshalkin A.B. [1], **Kaplun A.B.** [1], **Buzhdan Ya.M.** [2]

[1]- Institute of Thermophysics, kaplun@itp.nsc.ru

[2] Institute of Inorganic Chemistry, buzhdan@che.nsk.su

Earlier it was shown [1] that excess viscosity is the one-valued function of the interaction energy density $\Delta U/V$. It was shown [2] that well-known dependencies of viscosity on the state parameters (Arrhenius, Erring, Wargaftik, Doolitll) are special cases of the proposed in [1] equation. For calculation of the viscosity by the equation

[1] it is need to known the viscosity of hard sphere system by Enskog and dependence of the interaction energy on the state parameters. The viscosity gas and liquid in [1, 2] is calculated on the tabulated values of internal energy.

In paper the internal energy of substance is calculated using the well-known thermodynamic equation:

$$U(T,V)=\int\frac{RT^2}{V}\left(\frac{\partial Z}{\partial T}\right)_V dV+U_{ig}(T),\quad \Delta U(T,V)=U_{ig}(T)-U(T,V), \tag{1}$$

and compressibility factor $Z=PV/RT$ is write down as:

$$Z(T,V)=1+\frac{B(T)}{V}+\Delta Z(T,V). \tag{2}$$

The equation for second virial coefficient $B(T)$ described $B(T)$ of the wide variety of substances including helium and water was obtained by us with used of the combined spherically symmetrical potential of intermolecular interaction [3, 4]. It was found with a theories that $\Delta Z(T,V)$ is the one-valued function of the argument $x=1/(TV^3)$:

$$\Delta Z(T,V)=ax+bx^2. \tag{3}$$

The equation obtained with (1) - (3) to described coefficient viscosity of the wide variety of liquid and gas substances in wide range of temperature and pressure.

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WEIGHTED MONTE CARLO METHODS FOR SOLVING MANYPARTICLES PROBLEMS CONNECTED WITH THE BOLTZMANN EQUATION.

Mikhailov G.A., Rogasinsky S.V.
ICMMG gam@osmf.sscc.ru; svr@osmf.sscc.ru

With the general theory of the Monte Carlo methods [1,2], the new weighted modifications of a statistical modeling of evolution of the interacting particles ensemble related to the approximate solution of the Boltzmann equation are constructed. For this purpose, the special integral equation received on the basis of expansion of phase space of system by introducting the index of the realizing elementary interaction pair as the new coordinate into the phase space was used. It should be noted that construction of the standard weighted Monte Carlo estimators [1,2] on the basis the integral form of the master equation [3] is impossible, since its kernel represents the sum of mutually singular summands.

The weighted method can be used, for example, for redistribution on sorts of particles at t=0 with the purpose of the increase of frequency of modeling of the sorts of particles giving the basic contribution to the investigated functional. Also it is uneasy to increase frequencies of the most important pairs of interacting particles.

The weighted method enables effectively to study dependence of results on parameters of a task. In addition, it is possible to construct estimators of the appropriate parametric derivatives with a finite variance by the help of standard receptions of the weighted algorithms theory [1,2]. It is interesting to note, that it can be made on the basis of the direct modeling [1,2]. We shall note, that the probabilistic error of weighted estimators can be reduced by independent realizing the trajectories of system on separate computing processors with the subsequent averaging the received results.

By insignificant changes the stated technique can be distributed on a case when the sorts of particles can be changed, for example, as a result of chemical reactions.

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PROBLEM OF ISS CONTAMINATION – MODEL AND FULL SCALE EXPERIMENTS OF SERVICE MODULE REFUELLING LINES PURGE

Mishina L.V. [1]. Prikhodko V.G. [2], Chichenin A.G. [2], Yarygin V.N. [2], Yarygin I.V. [2]
[1]- S.P. Korolev RSC Energia, Lubov.V.Mishina@rsce.ru
[2]- Institute of Thermophysics, yarygin@itp.nsc.ru

Operation of various systems and devices of the International Space Station (ISS) is accompanied by periodic ejection of fuel components into space during the purging of fuel and oxidizer lines after refueling process. As the experiments previously conducted aboard the orbital station MIR have shown, the ejected components fall partially to the construction elements of the orbital station, resulting in their contamination, which is the negative factor. Recently the ISS contamination problem is under attention.

First results of comparison of the model and full-scale experiments of the Service Module refueling lines purging process researches are presented in this work.

Modelling of the real process of the lines purging was carried out in 1999-2000 at the Institute of Thermophysics SB RAS. This investigations, conducted in the vacuum installation for gas-dynamics researches VIKING, included in addition to methodological and methodical developments videoshooting of the flow structure and measurement of the droplet phase angular distribution during ejection of model liquids and gas-liquid mixtures into vacuum. Ultimate aim of this researches was to work-out recommendation for structural layout

of special protective system, which is to be mounted on the exit pipe of the fuel and oxidized lines in order to reduce the angles of the droplet phase ejection into vacuum and accordingly to decrease contamination of the ISS surface.

Full-scale experiment of the refueling lines was conducted in 2002 and included visual observation and videoshooting of the process of the fuel and the oxidizer ejection into vacuum. Obtained results were analyzed by Russian (RSC Energia) and American (NASA image science and analysis group) experts. Now we may speak about qualitative correspondence of model and full-scale experiments.

New problems and research settings in the field of rarefied gas dynamics concerned with the problem of orbital stations and space vehicles contamination are also considered in this paper.

PIC-DSMC SIMULATION OF WEAKLY IONIED GAS CLOUD EXPANSION BY PULSE LASER ABLATION

Morozov A.A., Plotnikov M.Yu.
Institute of Thermophysics, almoroz@itp.nsc.ru

The laser ablation of solid target by nanosecond pulses is considered for moderate laser intensity when surface evaporation takes place (0.1 – 2 J/cm^2). As a result of such a radiation, a cloud of low-temperature weakly ionized gas forms.

An effective tool for simulation of such a cloud expansion into vacuum is a combination of the direct simulation Monte Carlo (DSMC) method [1], which is used usually for calculation of neutral gas flows, and the Particle-in-Cell (PIC) method [2], which is used usually for collisionless plasma simulation. In the present work, a one-dimensional nonstationary problem with evaporation of particles (electrons, ions, and atoms) from the solid surface is considered. The Poisson equation is solved for describing of interaction between the charged particles. Collisions between ions and atoms are simulated. Dissociation and recombination is not taken into consideration. To determine the evaporation conditions (temperature at the surface and the number of evaporated particles), a thermal model for the target is used [3]. Special attention is given to exploration of effect of anomalous

plasma cloud acceleration due to charge space separation at the cloud front with the double layer formation [4]. The obtained results show anisotropic energy transfer from electrons to ions that results in a considerable acceleration of ions.

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DETERMINATION OF ACCOMMODATION COEFFICIENTS OF TRANSLATIONAL AND INTERNAL ENERGY OF MOLECULES OF GAS IN A FREE-MOLECULAR FLOWS

Morozov A.A., Plotnikov M.Yu., Rebrov A.K., Timoshenko N.I., Shishkin A.V.,
Institute of Thermophysics SB RAS, rebrov@itp.nsc.ru

The process of energy exchange between molecules of gas and a solid surface is of interest for researches by study of interaction of flight vehicles with atmosphere, development of technologies of sputtering on a surface and obtaining of thin films, study of heterogeneous relaxation of internal energy, research of catalytic processes etc. By these processes, the energy of incident molecules is an essential factor influencing on process of interaction with the surface.

From the literature, various methods of determination of accommodation coefficients of energy and momentum are known (AC)

[1,2]. In the present study a method based on the analysis of thermal condition of a thin wire for determination of accommodation coefficients of energy in a gas flow is proposed.

The developed technique was used for AC determination of various gases for the wire in a supersonic free-molecular flow. Among obtained results, negative AC values for internal energy for hydrogen, due to transfer of energy between translational and rotary degree of freedoms, is of particular interest.

The elaborated method of AC determination can be applied for measurements in gas mixtures also. At that, particular feature of adiabatic expansion of gas into vacuum is taken into consideration, that heavy components by collisions with easy component molecules are accelerated up to energies essentially exceeding stagnation energy of the heavy gas. The obtained values of AC of gas mixture components in a supersonic flow (M~10) are new ones and can be used for calculations of interaction of gas with a surface for technological devices and flight vehicles.

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THE MODEL OF GAS-KINETIC INTERACTION IN A PROBLEM OF AEROSOL PARTICLES DEPOSITION ON THE SURFACE

Pasechnik A.S., Beresnev S.A.
Ural State University, Sergey.Beresnev@usu.ru

The processes of aerosol particles deposition on and detachment from surfaces play an important role in the evolution of air-disperse system. The wide variety of deposition modes and conditions gives rise to numerous theoretical models and approaches to solution of the problem. The interaction of particles with a surface may be physical-chemical or electrostatic (including the effect of Van der Waals and

Coulomb forces), and well as gas-kinetic, similar to the hydrodynamic interaction. The characteristics of the gas-kinetic interaction of particles with the surface are not that thoroughly understood and studied as the characteristics of hydrodynamic interaction. A gas cannot be usually treated as continuum because of its rarefaction and molecular effects. The deposition processes usually proceed at widely varying gas pressure and temperature, and this leads to the particle-surface interaction different from that under continuum conditions. Actual atmospheric or technological processes involve a wide variety of gas-kinetic deposition modes: from the continuum mode to the mode of ultra rarefied gas; various inhomogeneities of gas medium caused by pressure, temperature and concentration gradients manifest themselves; particles may be under the exposure to external fields: gravitational, electrostatic or electromagnetic. The corresponding phoretic processes in aerosol (thermo-, diffusion-, electro-, turbo-, and photophoresis) are studied largerly within the model of aerosol particles in an unbounded gas volume. The presence of deposition surfaces gives rise to a wide variety of gas-kinetic effects and regularities that are studied rather fragmentarily and non-systematically yet.

The purpose of this study is an attempt to apply logically the gas-kinetic model of elementary processes of the particle-surface interaction with allowance for various inhomogeneities of the gas medium. The classification plans for deposition modes basing on introduction of three Knudsen numbers are considered. The opportunities of introduction in the model of other defining factors (for example, Brownian diffusion of particles) are analysed. The interrelation of used model for gas-kinetic interaction with known dynamic models describing the adhesion interaction, collision and detachment of particles from the surface is exhibited.

PERTURBATION NON-EQUILIBRIUM PROCESSES AT THE IMPACT SUPERSONIC FLOW DISTURBANCE CAUSED BY PERMEABLE OBSTACLE

Plotnikov M.Yu., Rebrov A.K.
Institute of Thermophysics, plotnikov@itp.nsc.ru

The submitted work is devoted to the research of features of the formation of one-dimensional supersonic gas flow through a permeable obstacle. The flow behind the obstacle remains supersonic at small disturbances. The macroparameters of this part of the flow are determined by the given thermal or momentum disturbance on the obstacle, as a matter of fact, by the given velocity distribution function of the molecules reflected from the obstacle. During the researches two models of the permeable obstacle were considered:

1. The molecules are reflected from a random distributed impenetrable part of the obstacle at a given permeability. Thus the reflecting surface of the obstacle is located perpendicularly to the gas flow.

2. The obstacle represents an infinite set of flat slits and plates of infinitesimal thickness. For the obstacle the Knudsen number was given according to the distance between the plates, and the width of the plate along the flow was given also. The calculations carried out by the method of direct statistical simulation [1] have shown an opportunity of solving such problem in any practical reasonable range of disturbances (a set of the velocity distribution functions of the reflected molecules). The calculations for concrete conditions have shown, that the limiting case of the transition from the supersonic flow to the subsonic one is characterized by the "stall", determined in the narrow limits of the disturbance variation.

The carried out researches within the framework of a four-parameters problem have allowed to determine a number of characteristic properties of the shock-wave disturbance formation at the interaction of a plane-parallel supersonic flow with the permeable obstacle, and also to determine the influence of the disturbance on the parameters of flow behind the obstacle. The submitted results allow concluding the opportunity of determination of the accommodation coefficient from the data on the macroparameters of the equilibrium flow behind the obstacle.

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IRRADIATIVE PROPERTIES OF THE CUMULATIVE JET, PRODUCED WITH THE EXPLOSIVE COMPRESSION OF THE COPPER CYLINDRICAL LINER

Pipich P.V.
Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Science, skin@hydro.nsc.ru

At explosive compression of a metal cylinder (liner) attached to a vacuum flask a specific cumulative jet is formed. The flow of metal vapors outflows in vacuum with the velocity up to 70 km/s – it is so-called high-velocity cumulative jet (HCJ). The basic jet goes after it with a smaller velocity. This jet consists of dispersed particles of the liner, in particular of copper clusters. The atoms and the clusters of copper are the consequence of a phase explosion of the liner. The described structure of the jet is the result of the jet studying with the help of a high-speed photo and the spectral analysis. The temperature of HCJ is determined with the measurement of the relative intensities of spectral lines. It is ~ 6000 K. The atoms concentration in the jet does not exceed 10^{18} sm^{-3}.

The kinetics of the population of the power levels of the copper atoms has been investigated in the extending jet with the help of a computer simulation. The change of the population was described by the system of differential equations, which took into consideration the influence of radiative processes, collision processes with participation of atoms, ions and electrons, and also radiation reabsorption on the population. The population of the copper atom levels follows the electron temperature exact enough (a deviation is no more than 20 %) and

therefore the determined value of the temperature can be considered true enough. The calculations have shown, that HCJ can serve as an active medium for the generation of laser radiation in yellow and green spectral regions. The big velocity of HCJ allows a fast change of the medium in a zone of generation, and provides the radiation continuity.

The radiative properties of the basic jet are defined by the presence of the clusters. The clusters as macroscopical particles absorb in the wide spectral region. Therefore the radiation of the cumulative jet sharply amplifies at the formation of clusters. The spectrum of the jet containing the clusters differs from the spectrum of continuous jet of the same material. Energy of a photon in the region of the radiation spectral power maximum of the small particle exceeds 1,2 times the maximal energy of a photon for black radiation at the given temperature. The cluster radiation is created by the radiation of all atoms, not by a surface radiation as in case of a continuous jet. In this respect the jet, consisting of the clusters, is an effective radiator. On the other hand, it follows from the equation of the balance of energy, connected to leaving radiation, for a unit of volume of the plasma, containing the clusters, that the cluster radiation does not contribute to the thermal balance of the extending jet, because the time of cluster radiation is small in comparison with the time of the jet expansion.

COPPER CLUSTERS FORMATION BY PHASE EXPLOSION OF CUMULATIVE JET

Pipich P.V.
Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Science, skin@hydro.nsc.ru

An explosive compression of a copper cylinder (usually named a liner) with the diameter of 12 mm and with the thickness of walls 1мм was studied experimentally. The liner had been attached to a vacuum flask. With the help of a high-speed photo and the spectral analysis it was found, that in the progress of collapse the copper vapor outflows in the vacuum with the velocity ~ 30 km/s (high-speed cumulative jet HCJ) is observed. The flow of the dispersed particles of copper (the basic jet) follows the vapors at a smaller velocity. The

spectral analysis of the gas component of the jet has shown, that the temperature of the HCJ equals ~6000 K.

The represented facts suppose the following interpretation. After initiation of an external explosion the collapse of the liner in the radial direction will occur. The process of the collapse is accompanied with intensive and fast (1-2 mks) heating of the internal layers due to viscosity of metal. The calculation shows that the temperature achieves thus several thousand K, and the specific thermal energy is comparable to the energy of explosives. There is a sharp increase of frequency of homogeneous nucleation, i.e. new phase nuclei appear due to the fluctuations. The system becomes unstable, when it achieves the phase transition spinodal, and the explosive transition to a two-phase state occurs. Thus the role of evaporation through a free surface thus is very small. There is the interpolating equation of copper state; the binodal and spinodal have been calculated according to this equation. As follows from the Laplace relation for the radius of drops the characteristic sizes of particles are $\sim 10^{-7}$ sm. The calculation has shown, that the cluster expansion velocity does not exceed 1 km/s. That is in agreement with the experimentally observed separation of the flow from the liner into the basic jet and HCJ.

The clusters can appear even after the removal of the external pressure after the expansion of the explosive products. The molecular dynamics simulation shows, that cavities appear in an expensing liquid, and then the transition to system consisting of the clusters and atoms is carried out.

MODELING OF THE PHYSICAL AND CHEMICAL PROCESSES ON THE SURFACES OF INTERSTELLAR GRAINS

Pyarnpuu A.A.[1], Cheredov V.V. [1], Shematovich V.I.[2]
[1]Moscow Aviation Institute
[2]Institute of Astronomy of the RAS

Both ion-molecular and neutral-neutral reactions with an activation energy are the very important chemical processes in the astrochemistry, but their kinetic rates are significantly lower than Langevin diffusion rate at the conditions characteristic for molecular clouds.

Usually it is suggested that kinetic rates of endoergic reactions could be significantly enhanced when the reacting molecules are in the excited state.

Interstellar matter concentrated in the clouds of cold rarefied gas is an open thermodynamic system which non-equilibrium state is determined by the energy inputs from external ultraviolet and corpuscular radiations. As a consequence of such influences the suprathermal and internally excited particles are produced in the dissociation and ionization processes, and in the exoergic chemical reactions.

In this paper the kinetics and dynamics of suprathermal and excited particles is described on the microscopic level by a set of nonlinear Boltzmann kinetic equations with source terms. In our previous studies it was found that in the cold molecular clouds hydrogen molecules (the main molecular constituent of interstellar matter) are

formed on the surfaces of interstellar grains and are efficiently ejected into gas phase with an excess of kinetic and internal energy.

The thermalization of initially hot hydrogen molecules through the collisions with ambient interstellar gas in the near-surface envelopes of interstellar grains is studied. The excess kinetic energy of ejected hydrogen molecules is varied from 0.1 eV up to 1.0 eV, and the elastic collisions with the ambient hydrogen gas are only considered with the characteristic collision cross section of 10-15 cm^{-2}.

Using the developed by authors modification of stochastic approach it was shown that hot hydrogen molecules ejected from the interstellar grains do not fully thermalize. Their steady state distribution functions by kinetic energy are characterized by the excess populations of molecules at the suprathermal energies. This can cause the enhanced role of endoergic reactions in the interstellar chemistry because the molecular hydrogen is a dominant constituent of the cold molecular clouds.

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OF A RAREFIED GAS STREAM AGAINST A WALL WITH DIFFERENT COEFFICIENTS OF ACCOMMODATION ON THE BASIS OF THE BOLTZMANN EQUATION

Raines A.A.
Saint Petersburg State University, raines@AR1063.spb.edu

We consider the unsteady problem of a rarefied gas stream against a wall with the mirror and diffusion laws of reflection with the complete accomodation (the piston problem). The first of these problems is considered as a test problem. The second one is interesting from the physical point of view, since one can observe processes related to the creation of the Knudsen wall layer and to the formation of the outgoing shock wave. The problem is studied for a binary gas mixture by the numerical solution of the Boltzmann equation. The collision integral is calculated by the conservative method of discrete velocities. This method was suggested for a simple gas in [1] and was generalized in [2] for a binary gas mixture and for the case of cylindrical symmetry. Conservativeness is provided without any restrictions on the admitted values of the variables of integration (for all possible collisions). The Boltzmann equation is solved by the splitting method (free-molecular flow and collisonal relaxation). For the first of these subproblems we use the divergence finite-difference scheme of the 2^{nd} order [3] and for the second one the Euler's method which provides satisfaction of conservation laws in each point x of the physical space. Numerical results are obtained by a modified algorithm based on the inclusion of the "inverse collisions". For the integration nodes we used the eight-dimensional grids [4].

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RAREFIED GAS DYNAMICS – RESEARCH FRONTIERS AND TRENDS

A.K. Rebrov
Institute of Thermophysics, rebrov@itp.nsc.ru

Rarefied gas dynamics was formed as separate field of kinetic theory and fluid mechanics mainly due to the start with a jerk of mankind into space with the extraordinary success in the very short historical time. Some scientific and practical base was founded to the beginning of that epoch. It was kinetic theory of gases and theory of rarefied gas flow in aspects of vacuum technologies.

The theoretical problems of flights in a rarefied atmosphere and practical questions of vacuum pumping in a very wide range of pressure for technologies (from about 10^4 to 10^{-8} Pa) to a considerable extent are solved to this time.

Now the research frontiers of rarefied gas dynamics are held over solution of problems of

- nonequilibrium processes at large gradients of parameters, characterized by local Knudsen number of order of 10^{-2} and higher,
- energy transfer in multi-temperature media, i.e. at an essential nonequilibrium on internal energy modes,
- description of processes in Knudsen layers in different situations on the boundary of gases with condensed medium,
- nano-mechanics of cluster atomic and molecular clots in gases, interaction of clusters, their behavior when interacting with surfaces.

Rarefied gas dynamics has a calling for study and describe breaks in continuum media flows on the level of account the real molecular interaction potentials. The true challenge for rarefied gas dynamics are:

- transition from a study of fluctuations to the level get to know the turbulence in open systems;
- description of nonequilibrium systems in dynamics related to modern high-tech processes;
- study of gas processes in micro- and nano-biological processes.

Methods of direct statistical simulation and molecular dynamics, enriched by adequate knowledge on interaction of molecules and clusters and realized by extremely growing computer possibilities apparently will become the main instrument for study of nonequilibrium processes in a wide range of energy nature. From the other side, the precision experimental studies of nonequilibrium phenomena will allow to determine unknown characteristics of molecules, their intercollisions and collisions with surfaces.

BOLTZMANN AND THE KINETIC THEORY. DYNAMICS, IRREVERSIBILITY AND DYNAMIC CHAOS

Rudyak V.Ya.
Novosibirsk State University of Architecture and Civil Engineering,
rudyak@ngasu.nsk.su

A hundred and thirty years have passed since the date of the issue of the basic works of L.Boltzmann. They played an important role in the radical change of our concept of the universe. On the basis of the Boltzmann's ideas the big interdisciplinary scientific trend including the kinetic theory, statistical mechanics, the theory of transport processes in gases, liquids and plasma, the theory of relaxation phenomena, statistical thermodynamics has been formed today. The significance of the Boltzmann kinetic theory is in the fact, that, perhaps, for the first time it showed the opportunity and necessity of various levels of description of many particles systems. For the last century science developed so rapidly, that not any obscurity should remain in the foundations of the kinetic theory. However this theory has raised such fundamental questions, many of which have no exhaustive answer till nowadays. That's why the analysis of the initial ideas, which L.Boltzmann laid in the foundations of his theory, is still far from having memorial significance. This is the point, which this work is devoted to.

In particular, the derivation of the kinetic equations of both rarefied and dense gases and the prospects of the kinetic description constructions for a liquid is being analyzed. In this connection the necessity of these or those statistical hypotheses, which are laid in the theory, is studied.

A well-known conflict between the reversible Hamilton descriptions of a many particles system and irreversibility of the Boltzmann kinetic description is a question of principle of the statistical theory. In the work the modern views on this problem having an important methodological and philosophical significance are discussed. In this connection, in particular, the correlation between the statistical description of many particles systems and the dynamic chaos, which takes place in such systems, is considered. It is shown, that the principal point of the dynamic and statistical description construction of many particles systems is the process of particles interaction. The classical mechanics, based on the concept of the material point, assumes, that this interaction is local and instant. This fact allows considering this interaction as a potential one. The potentiality of the forces of the particles interaction also results in the reversibility of the equations of mechanics. The opportunity of the construction of the kinetic equations on the basis of non-Hamiltonian equations of mechanics is discussed in conclusion.

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DYNAMIC AND STOCHASTIC PROPERTIES OF FINITE SYSTEM OF INTERACTING PARTICLES

Rudyak V.Ya., Ivanov D.A.
Novosibirsk State University of Architecture and Civil Engineering,
rudyak@ngasu.nsk.su

The work is devoted to the numerical study of the dynamic and stochastic properties of the systems of interacting particles. Various finite systems of the interacting hard disks placed in a two-dimensional volume have been considered. The interaction of the disks with each other and with a border was absolutely elastic. Thus, the considered systems are open; they exchange a momentum with the border. For the simulation of an equilibrium system the initial distribution of particles momentums was organized according to the Maxwellian distribution. For the given system the number of particles, density of the system and dispersion of the initial distribution of the

momentums (the temperature of the system) varied. As the finite volume a square and a round cells have been taken. In the first case the momentum and angular momentum were not constant in the system, in the second case only the momentum did not remain unchanged. The number of particles in the system accepted the values equal to 1, 2, 3, 5, 10, 50, 100, 1000. The systems, in which the following parameters did not remain constant were considered: (i) the momentum and the angular momentum, (ii) the momentum, (iii) the angular momentum. The purpose of the work was:

1. The study of reversibility of the phase trajectories of the system.
2. The study of the properties of stability of these trajectories concerning small variations of the initial data.
3. Determination of the parameters of instability, in particular, the Lyapunov exponent.
4. Determination of the relaxation times of the system.
5. The study of the dependence of the Lyapunov exponent and the relaxation times on the properties of the system (temperature, density, number of particles in the system).

It is stated, that the time of reversibility in the system is in the inverse proportionality to the number of particles and quickly decreases with the growth of the number of particle-particle collisions. Due to the special character of the law of particles interaction with the border, this interaction deforms poorly the character of the dynamic phase trajectories.

It is shown, that the phase trajectories are unstable. Generally there are some various regions of this dynamic curve; their evolution is described with different laws. However the region of local instability always takes place, when Δ increases exponentially at time. The autocorrelation functions of the particles velocity appear decaying. However the character of the decay essentially depends on the properties of the system. Thus, it is possible to ascertain the presence of dynamic chaos in the considered systems.

NANOPARTICLES DIFFUSION IN RAREFIED GASES

Rudyak V. Ya., Krasnolucki S.L.
Novosibirsk State University of Architecture and Civil Engineering,
rudyak@ngasu.nsk.su

Transport processes in rarefied ultradispersed gas suspensions with hard nanoparticles as dispersed component can be well described with the help of Boltzmann kinetic theory [1]. However it requires knowing an interaction potential of the dispersed particle with the carrier gas molecule. This potential was constructed in [2]. The aim of this presentation is a simulation nanoparticles diffusion coefficient in rarefied gas was on the basis of potential [2]. Dependences of the diffusion coefficient on radius of the dispersed particle and temperature of the carrier gas were studied.

It was shown that well-known Cunningham—Millikan—Davies experimental correlation has a sufficiently narrow temperature-application area. It is consistent with our calculation data within an accuracy of 15 % only in the temperature range from 100 to 300 K. At higher temperatures, it leads to strongly underestimated diffusion coefficient and, thus, cannot be applied [3].

Our second purpose was to obtain theoretical and experimental dependencies of diffusion coefficient on radius of nanoparticles and compare these dependencies with Cunningham—Millikan—Davies correlation. The last one is worldwide used for interpretation of results obtained with the Differential Mobility Analyser (DMA).

The experimental dependence of diffusion coefficient on radius of nanoparticles was obtained in the following way. Diffusion coefficient was measured with the DMA. Radii of nanoparticles distributions were obtained from Transmission Electron Microscopy (TEM) image measurements and calculated independently on the basis of the DMA data.

As a result of the theoretical and experimental data comparison it was established that in the small particle diameter area (less than 10 nm) the DMA method leads to large systematic error (it can be up to 100 % and more). It was bound up with use incorrect in this diameter area Cunningham—Millikan—Davies correlation in the DMA method. On the contrary the kinetic theory describes the nanoparticles diffusion experimental data at least with experimental precision [4].

This work was partly supported by the Russian Foundation for Basic Researches (grants No. 00-15-96164, No. 01-01-00045 and No. 02-01-06333).

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GENERALIZED H-THEOREMS OF BOLTZMANN FOR COMPLEX GAS MIXTURE

Rydalevskaya M. A., Tsibarov M. A.
Saint Petersburg State University

In this report the gas mixture with internal degrees of freedom and any chemical reactions including dissociation and recombination are considered. Side by side with the atoms and the molecules (Boltzmann particles) the elementary particles (Bose and Fermi) may be present. The properties of the functions $H_V(t) = -S_V(t)$ are investigated ($S_V(t)$ is the entropy of arbitrary gas volume V at time t).

The function $H_V(t)$ is submitted in the form

$$H_V(t) = \int_V \tilde{h}(\mathbf{r}, t) d\mathbf{r}, \qquad (1)$$

where $\tilde{h}(\mathbf{r}, t)$ is her density in the space of coordinates $\mathbf{r}$.

Using the results of statistical thermodynamics one may write

$$\tilde{h}(\mathbf{r},t)=\sum_i \int f_i \varphi_i d\mathbf{p}_i, \qquad (2)$$

$$\varphi_i = \ln\frac{f_i h^3}{s_i} - 1, \qquad i \in Boltz, \quad (3)$$

$$\varphi_i = \frac{s_i}{f_i h^3}\ln\frac{s_i}{f_i h^3} - \left(\frac{s_i}{f_i h^3}+1\right)\ln\left(\frac{s_i}{f_i h^3}+1\right), \qquad i \in B, \quad (4)$$

$$\varphi_i = \left(\frac{s_i}{f_i h^3}-1\right)\ln\left(\frac{s_i}{f_i h^3}-1\right) - \frac{s_i}{f_i h^3}\ln\frac{s_i}{f_i h^3}, \qquad i \in F. \quad (5)$$

Here $f_i(\mathbf{r},\mathbf{p}_i,t)$ is a distribution function in the space of impulses $\mathbf{p}_i$; i corresponds to the set of indices which determine chemical sort and quantum levels of energy for the particle; h is the Plank's constant; s_i is the statistical weight; $i \in Boltz$, $i \in B$ and $i \in F$ correspond to the particles of Boltzmann, Bose and Fermi.

The formulas (1)—(5) and the generalizations [1,2] of classical Uehling-Uhlenbeck equations allow to prove some theorems.

Theorem 1. *For uniform space gas mixture the inequality* $d\tilde{h}/dt \le 0$ *is true.*

Theorem 2. *For arbitrary considered gas mixture the inequality* $dH_V/dt \le \Delta H_V$ *is true (*ΔH_V *is a change off* H_V *owing to a flux of the values* φ_i *trough the surface into the volume V).*

Theorem 3. *For arbitrary considered gas mixture the inequality*

$$\frac{\partial \tilde{h}}{\partial t} + \mathrm{div}(\tilde{h}\mathbf{v}) + \mathrm{div}\,\mathbf{q}_\varphi \le 0 \qquad (6)$$

is true. Here $\mathbf{v}$ *is mass velocity of the mixture,,* $\mathbf{q}_\varphi = \sum_i \int f_i \varphi_i \mathbf{c}\, d\mathbf{c}$ *is a flux vector of the values* φ_i, $\mathbf{c}$ *is peculiar velocity of the particle.*

In particular case of local eqilibrium the inequality (6) turns into equality

$$\frac{\partial \tilde{h}}{\partial t} + \mathrm{div}(\tilde{h}\mathbf{v}) = 0. \qquad (7)$$

Equation (7) corresponds to isoentropic flows of gas mixtures.

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GROUP THEORY APPROACH AND NEW RENORMALIZED FORM OF BOLTZMANN EQUATION.

Saveliev V.L.

Institute of Ionosphere , Alma-Ata, saveliev@hotmail.kz

Boltzmann equation forms a basis of kinetic plasma and gases description. To write down a collision integral in this equation the author suggests to parameterize a process of collision by a rotation matrix and then make use of the construction of *invariant integration over a group*. This parameterization provides that the transformation of velocities due to collision becomes linear one and that the collision matrixes constitute the *collision group*. With the help of construction of *representation* of this group in the Hilbert space of two particles distribution functions it becomes possible in a simple way to exactly renormalize the Boltzmann collision integral. Due to this, in particular, the long standing problem in the kinetic theory, how to effectively describe in the frame of the Boltzmann equation the dynamic of particles interacting with long range potentials, have been solved. A new renormalized form of Boltzmann kinetic equation has a form of Liouville equation with the nonlocal friction force, which depends on the distribution functions of the gas mixture (plasma). This new equation allows us to think about the searching distribution function as a density of points (hypothetical particles) in the face space, which are

moving along the smooth trajectories and do not jumping any more, as it was in the case of the classical Boltzmann equation. This fact opens new opportunities for the direct modeling of gas dynamic and plasma kinetic problems.

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ABOUT ANALYTICAL KINETIC EQUATION SOLUTION IN THE PROBLEM OF POINT SOURCES IN POLYATOMIC GAS

Savkov S.A., Yushkanov A.A., Yalamov Yu.I.
Orel State University,
Moscow State Regional University,
yushkanov@mtu-net.ru

The analytical solution of the BGK model analogue of the kinetic equation for a point source of heat or particles in polyatomic gas is obtained. The analysis of energy and temperature distribution on translational and rotational degrees of freedom of molecules is carried out at their separate excitation.

The solution is carried out in three stages: we consider the kinetic equation for an infinite plane source of the given phase density and we search for the particular solutions of the corresponding homogeneous equation by the Case method. These solutions compose a full system of orthogonal functions. Further, we expand the distribution function in the obtained system of functions and determine macroscopical parameters of gas. After that, using the connection between solutions for a plane and spherical geometry, we find the distribution of corresponding values from the isotropic point source.

It is shown, that the obtained results translate into the well-known gas dynamics expressions on the distances about ten mean free paths. Quite near the source the temperature and concentration values change in inverse proportionality to the square of the distance from the source. Thus in case of the source of heat the rotational degrees of freedom give a little bit greater contribution to the temperature distribution, than the translational degrees, and in case of the particles source the basic change of internal energy of molecules is caused by their translational movement. And, the difference from the results of gas dynamics solution is a little bit less than the difference from the solution for one or two-atomic gases.

The obtained results can be used both at the general analysis of the heat transfer and mass transfer processes in molecular gases, and for the solving of concrete problems. For example, these results can be used for the study of the thermal effects of the interaction of laser radiation with substance; that is especially actual at the research of the self-focusing and defocusing of the laser beam in the absorbing medium.

BOLTZMANN EQUATION FOR ELECTRON DISTRIBUTION FUNCTION REVIEW OF LOCAL AND NON-LOCAL METHODS OF SOLUTION

Sukhinin G.I., Fedoseev A.V.
Institute of Thermophysics, sukhinin@itp.nsc.ru

In the paper, the review of the state of the art solution of the Boltzmann Equation (BE) for electron energy distribution function (EEDF) is presented. Special attention is given to the problems of solution of non-local Boltzmann Equation and description of stratified states in low-temperature plasma.

The history of the development of the solution methods of BE for EEDF counts almost a hundred years starting with the work of H.A. Lorentz, and can be divided in several periods.

1. *Early works of the first half of the 20th century* (Druyvesteyn, Davydov, Allis, Holstein and others). Expansion of EEDF in a series of spherical harmonics was introduced. Boltzmann equations for isotropic and anisotropic parts of EEDF were obtained. Solutions for homogeneous plasmas in the uniform constant or RF electric fields were obtained in two term approximation.

2. *Development of solution methods of BE and accumulation of data on electron-molecule cross sections* in the 60-80s of the 20th century, *concerned first of all with the research in laser physics and MHD.* Inelastic collisions were taken into account. Reliable information on electron transport coefficient depending on reduced electric field was obtained (L.G.H.Huxley, R.Crompton L.S.Frost, A.V.Phelps, A.Kh.Mnatsakanyan, R.I. Lyagushchenko, A.P. Napartovich, A.A. Kudryavtsev, L.D. Tsendin, and others).

3. *Research of EEDF devoted to the solutions of applied plasma chemical problems* was started in the 80s of the 20th century (L.D. Tsendin, V.A. Godyak, V.I. Kolobov, V.A. Shveigert, A.V.Phelps, L.Pitchford, J.-P.Boeuf, P. Segur, U. Kortshagen, M.Kushner, and others). There took place an impetuous development of numerical solution methods of BE for different applications and active use of Monte Carlo and Particle in cell (PIC/MC) methods.

In the current decade, methods of solution of the non-local BE, different hybrid methods, and self-consistent approaches to the solution of spatially non-homogeneous and stratified low-temperature plasmas are being actively developed (R.Winkler, F. Sigeneger, D. Uhrlandt, L.Pitchford, J.-P.Boeuf, C.Ferreira, L.L. Alves, A.Bogaerts, Z. Donko, L.D. Tsendin, Yu.B. Golubovskii and others).

As examples of solutions of non-local BE, the problem of secondary electrons distribution function generated in gases by high-energy electron beam, and the problem of spherical stratified low-pressure glow discharge are considered.

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FIRST ORDER PHASE TRANSITION IN CLUSTERS

Umirzakov I.Kh.
Institute of Thermophysics of the Siberian Branch of the Russian Academy of Science, umirzak@online.sinor.ru

It is known, that clusters have a set of various stable configurations of atoms (molecules). Each stable configuration of atoms is named the cluster isomer. A point of minimum on the surface of cluster potential energy corresponds to every isomer. This point is characterized with the value of the potential energy and a surface curvature in this position. Each point of the minimum has the domain of attraction on the surface of potential energy (catcment basin), which contains a unstable configurations of cluster atoms. Each unstable configuration transits into the given stable configuration at the cluster cooling. Obviously, the properties of the potential energy surface determine all physical properties of the clusters.

In the work the connection of the properties of the phase transitions solid - gas and liquid - gas in a finite system with characteristics of the catcment basin of the system potential energy surface is investigated. The influence of a spectrum of isomers and anharmonicity of vibration on the properties of the phase transitions is considered.

For the first time the potential energy surface model, which results in occurrence of a horizontal site on the p-V-diagram a thermodynamic limit (mathematically strict phase transition), is proposed.

NEW METHOD OF PAIR INTERACTION POTENTIAL DETERMINATION

Umirzakov I.Kh.
Institute of Thermophysics of the Siberian Branch of the Russian Academy of Science, umirzak@online.sinor.ru

The interaction of molecules (atoms) is known to play a key role in determination of properties of rarefied gases, and the study of

characteristics of this interaction is one of the primary problems of molecular physics.

In the work a new method of determination of the pair radial potential of the molecular (atom) interaction is proposed. This method is based on the analysis of experimental data on the dependence of the second virial coefficient on temperature.

The given method allows determining the interaction potential with any given accuracy and has clearer and stricter mathematical basis, than other similar methods.

Testing of the method for Morse and Lenard-Jones potentials is discussed, and also the results for the inert gases and a number of nonpolar substances are represented. The results are compared with the data found in scientific literature.

NEW MODEL FOR ACCOUNTING OF ANHARMONICITY OF CLUSTERS VIBRATIONS

Umirzakov I.Kh., Chekmarev S.F.
Institute of Thermophysics of the Siberian Branch of the Russian Academy of Science, umirzak@online.sinor.ru

It is known, that the surface of potential energy of clusters can be submitted as a set of domains of attraction to the points of minima of this surface (catcment basins). A stable configuration of cluster atoms (molecules), named the isomer, corresponds to each point of the minimum. Each point of catcment basin of the given isomer corresponds to the certain unstable configuration of atoms.

At low temperatures the movement of atoms in the cluster is described by a set of linear vibrations, and at high temperatures anharmonicity effects become dominant.

In the work the new approximation (model) of the catcment basins of the cluster isomers for the account of anharmonicity of vibration have been proposed. The characteristics of the catcment basins are determined from properties of the atom interaction potential and consequently the model does not contain adjustable parameters.

It is shown, that the given model gives a good quantitative description of the dependence of average kinetic energy on full energy on the clusters isomers consisting of 13 atoms of argon, xenon or krypton. This dependence was acquired by the taboo search method, developed by S.F.Chekmarev and S.V.Krivov.

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FLUCTUATION OF THERMODYNAMIC VARIABLES IN SMALL OPEN SYSTEM

Kharlamov G.V., Rudyak V.Ya.
Novosibirsk State University of Architecture and Civil Engineering, rudyak@ngasu.nsk.su

The fluctuations of density, momentum and energy play a determining role for the transport processes in dense gases and liquids. The statistical theories of small fluctuations advanced by A.Einstein and J. Gibbs, result in the Gauss distribution functions of thermodynamic parameters. However, these theories are available only for a big number of molecules in the system. The recent rapid development of nanotechnologies, physics and chemistry of aerosols and colloid systems, microbiology and biophysics results in the necessity of considering the fluctuations of density, momentum and energy in small volumes of gases and liquids. In works [1,2] it is shown, that the fluctuations of the momentum in small volumes cardinally influence diffusion of nanoparticles in dense gases and liquids. The fluctuations in small subsystems are not small and the theory of such fluctuations is not yet developed. The construction of such theory also is the purpose of the annotated work.

The statistical theory of the fluctuations of a number of particles, momentum and energy in the small open subsystems being a part of a big thermodynamic system is offered. The description of such fluctuations is carried out on the basis of the A.Einstein's modified theory, in which the expansion of entropy into fluctuation series is not used, as these fluctuations of thermodynamic values are not small. The advanced theory results in the essentially non-Gauss character of distri-

bution functions of a number of particles and energy at a small average value of the particles number N_0 in the subsystem. At a big N_0 the distribution functions of thermodynamic values translate in the Gauss functions. In this case the dispersion of these distributions coincides with the dispersion received in the theory of small fluctuations of A.Einstein.

The constructed distribution functions of a number of particles, momentum and energy are compared then to the results of numerical simulations by the molecular dynamics method. The good agreement of the theoretical distribution functions and the histograms of the distribution of the thermodynamic values, received in the numerical experiment, is observed.

Further in the work the results of the simulations of the relaxation of thermodynamic fluctuations in small open systems by the molecular dynamics method are presented. Two regions of the time dependence of the autocorrelation function of the thermodynamic fluctuations are revealed: a fast exponential one and a slow non-exponential one. The mechanisms of the relaxation of the considered fluctuations are discussed.

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HEURISTIC MOLECULAR DYNAMICS AND ITS APPLICATION TO THE STUDY OF CLUSTERS AND BIOMOLECULES

Chekmarev S. F.
Institute of Thermophysics, chekmare@itp.nsc.ru

A new, *heuristic* approach to the computer simulation study of complex many-body systems is presented. Unlike the existing approaches, it does not pursue a goal of reproduction of inherent dynamics and statistics of the system. Instead, using information obtained to the current moment, a guided exploration of the potential energy surface (PES) is made, with the results of the simulation allowing a reconstruction of the inherent behavior of the system. For this purpose, the molecular dynamics (MD) trajectory of the system is confined to the catchment basins on the PES that correspond to the structures of interest (isomers and conformers) [1-4]. The approach reduces the computational efforts radically, and at the same time it allows one to perform not only a detailed study of individual structures [2-4] and their interconversion [1, 3, 4], but a complex study of a system, including surveying the PES and calculating the equilibrium properties and kinetics [5-7]. In the latter case, following a suitable 'taboo-search' strategy of surveying the PES, the system is confined successively to various catchment basins on the PES.

Due to this approach, many problems that were a challenge to computer simulation study have become tractable: the investigation of properties of individual isomers (Lennard–Jones clusters [2-4]) and rates of complex transitions (carbon clusters [1, 3, 4]), surveying complex PESs ((Lennard–Jones clusters [6] and oligopeptides [5]), and the *ab initio* MD study of kinetics of metallic clusters (gold clusters [7]).

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HEAT EXCHANGE AND PHOTOPHORETIC FORCES IN AEROSOL AGGREGATES IN FREE-MOLECULAR REGIME

Cheremisin A.A.
Krasnoyarsk State Technical University,
cheremisin@nifti.krasnoyarsk.ru

Since the work [1] a large number of works are devoted to the thermophoretic and photophoretic motion of aerosol aggregates in gas substances in near-continuum Knudsen number limit. Meanwhile, in the upper atmosphere the aerosol particles are in comparatively rarefied gas medium. It is assumed that the photophoretic forces play an important part in vertical transport of soot particles into the upper atmosphere [2]. It may be assumed that for solution of the problem of aerosol stratification in the upper atmosphere [3] the photophoretic effects are to be taken into account.

At present the quantitative theory of photophoretic forces is well advanced for ideal spherical aerosol particles only. Two mechanisms of the forces inducing are known. They are the relatively weak ΔT-photophoresis [4,5] and the strong $\Delta\alpha$-gravito-photophoresis [2].

In this report a heat exchange and photophoretic forces calculation procedure, based on the Monte-Carlo method, for the complex aggregated aerosol particles in the free-molecular regime is presented. The calculations for monospherical and bispherical aerosol particles in conditions of standard atmospheres [6] have been carried out to date. The new strong mechanism of photophoretic forces inducing in aerosol aggregates – ΔT-gravito-photophoresis is revealed. A connection between the gravito-photophoretic forces and the structure of aerosol scattering in the middle and upper atmosphere is shown.

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EVALUATION OF THE COLLISION OPERATOR FOR A GAS WITH INTERNAL DEGREES OF FREEDOM

Cheremisin F.G.
Computing Centre of RAS, tcherem@ccas.ru

A method for evaluation of the collision operator of the generalized Boltzmann (Wang Chang – Uhlenbeck) equation that describes a gas with internal degrees of freedom is proposed. The considered method presents an extension of the conservative projection method for the Boltzmann collision integral previously developed by the author [1]. For any accuracy of calculations determined by the used descretization grid and by a number of nodes of the integration formula, it guarantees the preservation of the sum of the internal and the translational energies and a correct balance of these energies at the thermodynamic equilibrium state. The cases of degenerated rotational spectra and of not degenerated vibration one are considered. Some examples of solutions of the Wang Chang – Uhlenbeck equation are given.

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SOLUTION OF THE BOLTZMANN EQUATION AT SMALL KNUDSEN NUMBERS

Cheremisin F.G.
Computing Centre of RAS, tcherem@ccas.ru

It is essential for solving the Boltzmann equation at low Knudsen numbers, that a numerical error of calculation of the collision integral be substantially bellow of the value of the integral determined by a small deviation of the solution from a local maxwellian distribution function. Such condition is satisfied in the method of [1] in which the collision integral from maxwellian function is exactly equal to 0 independently on numbers of nodes of the velocity and of the integration grids.

The kinetic equation is solved by a method of splitting on a free molecular and a relaxation stages. The differential operator is approximated by a second order finite difference scheme. At the relaxation stage a second order scheme of the predictor-corrector type could be applied. For steady problems an acceleration of the convergence to the solution can be obtained by the inclusion in the algorithm of the gas dynamic stage in which Euler equations are solved by a kinetic method. Some methodical calculations are reported.

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LIGHT INDUCED EVAPORATION AND AEROSOL GROWTH

Chernyak V.G., Klitenik O.V.
Ural State University,
vladimir.chernyak@usu.ru

The light induced aerosol particle evolution, connected with radiation absorption by the particle and by vapor molecules selectively on their velocities, has been investigated.

The spherical particle, suspended in a mix of its vapor and not condensed gas, is irradiated with the light, which represents a running plane monochromatic wave. At the absorption of light the particle is heated up and starts to evaporate (radiometric evaporation).

Let the frequency of the running light wave is close to an absorption line on electronic or vibrational-rotational transition of the vapor molecules. Due to the Doppler effect only those vapor molecules, which velocities projections to a direction of radiation propagation have values in a certain narrow interval, can absorb the light and be excited. The excited molecules change their transport properties — in particular, collision cross-section. The velocity distribution function of vapor molecules becomes nonequilibrium. As a result the vapor temperature becomes distinct from temperature of vapor-gas mixtures (resonant heating or cooling of vapor). If the vapor temperature is higher than the equilibrium temperature of the vapor-gas mixture, the particle evaporates. Otherwise growth by the condensation takes place.

The difference of coefficients of evaporation - condensation for the excited and not excited vapor molecules is also the reason of evaporation or growth of the particle. If the condensation coefficient of the excited molecules increases, the process of condensation becomes prevailing and the particle grows.

The distribution functions of the excited and not excited vapor molecules, and also of buffer gas molecules satisfy to system of Boltzmann equations. The distribution of temperature in the particle is described by the inhomogeneous heat conduction equation.

The size of the particle was much less than the mean free path of molecules in the gas phase, i.e. the free-molecular regime was considered.

As a result the expressions for the kinetic coefficients, describing surface and volumetric mechanisms of evaporation (growth) rate of the aerosol particle have been received. The dependence of these coefficients on the value of the radiation frequencies detuning from the center of the absorption line has been investigated. It has been ascertained, that the evaporation (condensation) rate is maximal at the exact resonance. The direction of the process, i.e. evaporation or growth of the particle, is (determined) by signs on differences of effective di-

ameters of the excited and not excited vapor molecules, their coefficients of evaporation and the absolute value of detuning.

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SPECIFIC FEATURES OF GAS KINETICS IN A RESONANT RADIATION FIELD

Shalagin A.M.

Institute of Automation Electrometry, shalagin@iae.nsk.su

There presented a review of notions and ideas of kinetics of resonantly irradiated gas systems. As it had appeared this kinetics demonstrated drastically unexpected features. For example, the friction force may behave strange - it does not merely decelerate any relative motion of gas components, but rather create it. The velocity of fluxes may be up to the sonic one. This phenomenon is known as light-induced drift (LID). The common feature of the majority of new phenomena is the transformation of randomness into order without any work of creation of "Maxwellian demon". Many physicists as dubious have considered even the idea of such a device.

On the basis of LID and related phenomena the separation of gas mixture components (in particular, isotopes and nuclear isomers separation) have been realized. Valuable information on atomic and molecular collisions as well as on intramolecular processes was obtained. It is worth to note the role of light-induced drift and the so-called light-induced current (LIC) in astrophysics: LID is considerably responsible for separation of chemical elements and isotopes stellar atmospheres of peculiar stars and protoplanet clouds. LIC may appear to be among the sources of solar magnetic field.

ANALYSIS OF ACCURACY OF NUMERIC SOLUTION OF GAS DYNAMICS PROBLEMS BY DIRECT STATISTICAL SIMULATION METHOD

Shevyrin A.A., Bondar E.A., Ivanov M.S.
Institute of Theoretical and Applied Mechanics of the Siberian Branch of Russian Academy of Science, shevr@itam.nsc.ru

At the direct statistical simulation (DSS) of rarefied gas flows the estimates of the numerical calculation accuracy is necessary. In case of flows at Knudsen numbers Kn ~ 1 (transition regime) a series of calculations is usually executed with mesh refinement and with increase of the number of model molecules till acquiring the numerical solution convergence. The DSS calculations of flows in circumcontinual regime (at Knudsen numbers equal Kn<<1) require essentially large computing resources, and often the numerical solution convergence cannot be shown for such problems. That's why for such regime the accuracy of the acquired numerical solution is an especially important question, i.e. how much this solution deviates from the Boltzmann equation solution.

In the calculation methods of the continual gas dynamics the problem of the numerical error analysis is well studied, and there are different ways of estimates execution of the numerical solution accuracy. Similar analysis for the DSS method has not been done till nowadays. The complexity of such analysis is connected with different errors, which may be divided into the errors due to finiteness of the number of model molecules, and errors due to time and space discretization.

A finite number of the model molecules is used in the DSS method, and therefore there is always a statistical dependence between them. The presence of the statistical correlations means that the molecular chaos condition, used for the derivation of the Boltzmann equation is broken. In present work the relationship between the statistical dependence and the deviation of the numeric solution from the Boltzmann equation solution is studied. Two ways are offered for the estimation of the statistical correlations value: determination of the relative number of the recurring collisions and calculation of the correlator G_2 of the type $\langle v_1^2 v_2^2\rangle / \langle v_1^2\rangle\langle v_2^2\rangle - 1$. Proximity of these parameters to zero means a low level of statistical dependence between the model particles. Three classical problems of gas dynamics were considered with the main features, characteristic of complicated flows of rarefied gas reviled in them: the problem of internal structure of the shock wave, the problem of Couette flow and the problem of heat transfer between two parallel plates. The main result of the investigation is the determination of the maximum limits of values of the relative number of secondary collisions and the correlator G_2, for which the contribution of statistical correlations in the macroparameters values is acceptable. The influence of time and space discretization on the error of the numerical solution is also studied in present work. Multiparametrical investigations have been done for all three abovementioned problems, while the number of model molecules the parameter of time step and the size of collision sells had different values. An interesting result is an essential increase the error of time discretization with the increase of statistical correlations between the model particles.

A STUDY ON THE COLLISION INTEGRAL FOR THE ORIENTED PARTICLES

Ender A.Ya., Ender I.A.
St.-Petersburg Physico-Technical Institute,
St.-Petersburg State University
andrei.ender@pop.ioffe.rssi.ru

Previously, the present authors investigated the matrix elements (ME) of the Boltzmann collision integral for the distribution function, the latter being isotropic and axially symmetric over the velocities. It was shown that the nonlinear matrix elements of the collision operator are interrelated via the simple relationships, these relationship being valid for the arbitrary cross sections of the particles' interactions even with a preferred direction in a space. These relationships were deduced from an invariance property of the collision operator relative to a choice of the basic functions. As the basis it was assigned a set of the spherical Hermite polynomials with a Maxwell weight function;

and its invariance relative to the changes in the temperature and average velocity of the weighted Maxwellian was applied.

In a general 3D case, the Hermite polynomials contain the real spherical harmonics $Y^i_{l,m}(\theta,\varphi)$, ($i=0$ refers to $\cos m\varphi$, a $i=1$ - $\sin m\varphi$) depended on two angles θ and φ. Now, a transition from a given basis to another refers to the rotation angle ω around Z-axis or ψ around Y-axis. New recurrent relations between MEs are generally a set of the differential equations.

Essentially new results are obtained when a system has a preferred direction and there are oriented particles. The particles become oriented, e. g., in a strong electrical or magnetic field. For these particles, there are no constrains on MEs introduced by a Hecke theorem and its generalization in a non-linear case. A number of new effects arise which have not any explanation within the standard kinetic theory. From the constructed systems of the differential equations we successes in seeking the new relations describing the kinetic coefficients for asymmetric oriented particles and in determining how each matrix element can depend on the rotation angles.

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EXPANSION OF A KERNEL OF NONLINEAR COLLISION INTEGRAL OVER SPHERICAL HARMONICS

Ender A.Ya., Ender I.A.
St.-Petersburg Physico-Technical Institute,
St.-Petersburg State University
andrei.ender@pop.ioffe.rssi.ru

In our works it was built a set of the universal recurrence relationships for the matrix elements (ME) as the linear as the non-linear ones of the collision intgral. For the central simmetric potentials (non-oriented particles) there are additional relations between the linear MEs (integral brackets) giving an opportunity to express any ME via the isothropic linear diagonal MEs. This statement is a corollary of a

Hecke theorem. Now it is a way to calculate the non-linear MEs with large indices.

Hilbert constructed analytically a kernel of the collision operator for a hard-sphere model. Hecke expansed this linear operator kernel over the spherical harmonics. In this paper shown is how to construct the analogous expansion for the arbitrary cross sections and non-linear case when using the known MEs. The kernels obtained give an opportunity to construct the equations for the expansion coefficients over the spherical harmonics. This method is free from constraints on distribution function inherent to the Grad criterion. It is shown, also, how it can be used a kernel expansion in solving the boundary problems with discontinuous distribution functions.

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